

Causal inference in partially linear structural equation models: identifiability and estimation

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Abstract: We consider the identifiability and estimation of partially linear additive structural equation models with Gaussian noise (PLSEMs). Existing identifiability results in the framework of additive SEMs with Gaussian noise are limited to linear and nonlinear SEMs, which can be considered as special cases of PLSEMs with vanishing nonparametric or parametric part, respectively. We close the wide gap between these two special cases by providing a comprehensive theory of the identifiability of PLSEMs by means of (A) a graphical, (B) a transformational, (C) a functional and (D) a causal ordering characterization of PLSEMs that generate a given distribution \mathbb{P} . In particular, the characterizations (C) and (D) answer the fundamental question to which extent nonlinear functions in additive SEMs with Gaussian noise restrict the set of potential causal models and hence influence the identifiability.

On the basis of the transformational characterization (B) we provide a score-based estimation procedure that outputs the graphical representation (A) of the distribution equivalence class of a given PLSEM. We derive its (high-dimensional) consistency and demonstrate its performance on simulated datasets.

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1. Introduction

Causal inference is fundamental in many scientific disciplines. Examples include the identification of causal molecular mechanisms in genomics [22, 23], the investigation of causal relations among activity in brain regions from fMRI data [18] or the search for causal associations in public health [7].

A major research topic in causal inference aims at establishing causal dependencies based on purely observational data. The notion “observational” commonly refers to the fact that one obtains the data from the system of variables under consideration without subjecting it to external manipulations. Typically, one then assumes that the observed data has been generated by an underlying causal model and tries to draw conclusions about its structure.

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Two main research tasks in this setting are identifiability and estimation of the underlying causal model. In this paper we address both of them for partially linear additive structural equation models with Gaussian noise (PLSEMs). So far, there exists a wide “identifiability gap” for PLSEMs, as their identifiability has only been characterized for the two special cases where all the functions are linear or all the functions are nonlinear. We close this “identifiability gap” by providing comprehensive characterizations of the identifiability of the general class of PLSEMs from various perspectives.

Unlike in regression where partially linear models are mainly studied because of efficiency gains in estimation, the use of partially linear models has a deeper meaning in causal inference. In fact, as we will show, it is closely connected to identifiability. The functional form of an additive component directly influences the identifiability of the corresponding (and also other) causal relations. For this reason we strongly believe that the understanding of the identifiability of PLSEMs is important. First and foremost, it raises the awareness of potentially limited (or increased) identifiability in the presence of linear (or nonlinear) relations in the data. Second, by not restricting the functions to be either all linear or all nonlinear, PLSEMs allow for a flexible modeling approach.

We start by reviewing and introducing important concepts in Section 1.1. We then provide a brief overview of related work in Section 1.2 and explicitly state the main contributions of this paper in Section 1.3.

1.1. Problem description and important concepts

We consider p random variables $X = (X_1, \dots, X_p)$ with joint distribution \mathbb{P} , which is assumed to be Markov with respect to an underlying directed acyclic graph (DAG). A DAG $D = (V, E)$ is an ordered pair consisting of a set of vertices $V = \{1, \dots, p\}$ associated with the variables $\{X_1, \dots, X_p\}$, and a set of directed edges $E \subset V^2$ such that there are no directed cycles. A directed edge between the nodes i and j in D is denoted by $i \rightarrow j$. Node i is called a *parent* of node j and j is called a *child* of i . Moreover, the edge is said to be oriented *out of* i and *into* j . If $i \rightarrow j$ or $i \leftarrow j$, i and j are called *adjacent* and the edge is *incident* to i and j . The *degree* of a node i , denoted by $\deg_D(i)$, counts the number of edges incident to node i in DAG D . A node k that can be reached from i by following directed edges is called *descendant* of i . We use the convention that any node is a descendant of itself. The set $\text{pa}_D(j) = \{i \mid i \rightarrow j \text{ in } D\}$ consists of all parents of node j . The multi-index notation $X_{\text{pa}_D(j)}$ denotes the set of variables $\{X_i\}_{i \in \text{pa}_D(j)}$. An edge $i \rightarrow j$ is said to be *covered* in D , if $\text{pa}_D(i) = \text{pa}_D(j) \setminus \{i\}$. In that case, $\text{pa}_D(i)$ is a *cover* for edge $i \rightarrow j$. The process of changing the orientation of a covered edge from $i \rightarrow j$ to $i \leftarrow j$ is referred to as a *covered edge reversal*. A triple (i, j, k) is called a *v-structure*, if $\{i, j\} \subseteq \text{pa}_D(k)$ and i and j are not adjacent. The graph obtained by replacing all directed edges $i \rightarrow j$ by undirected edges $i - j$ is called *skeleton* of D . The *pattern* of a DAG D is the graph with the same skeleton as D and $i \rightarrow j$ is directed if and only if it is part of a *v-structure* in D . A permutation $\sigma : V \rightarrow V$ is a *causal ordering* of D

if $\sigma(i) < \sigma(j)$ for all $i \rightarrow j$ in D . DAGs may be used as underlying structures for structural equation models (SEMs). A SEM relates the distribution of every random variable $\{X_1, \dots, X_p\}$ to the distribution of its direct causes (the parents in the corresponding DAG D) and random noise. In its most general form,

$$X_j = f_j(X_{\text{pa}_D(j)}, \varepsilon_j), \quad j = 1, \dots, p, \quad (1.1)$$

where $\{f_j\}_{j=1, \dots, p}$ are functions from $\mathbb{R}^{|\text{pa}_D(j)|+1} \rightarrow \mathbb{R}$ and $\{\varepsilon_j\}_{j=1, \dots, p}$ are mutually independent noise variables. Lastly, for a function $F : \mathbb{R}^p \rightarrow \mathbb{R}^p$, we write DF for the Jacobian of F .

1.1.1. Main focus: PLSEMs

In this paper we study the restriction of the general SEM in equation (1.1) to *partially linear additive SEMs with Gaussian noise (PLSEMs)* of the form:

$$X_j = \mu_j + \sum_{i \in \text{pa}_D(j)} f_{j,i}(X_i) + \varepsilon_j, \quad (1.2)$$

where $\mu_j \in \mathbb{R}$, $f_{j,i} \in C^2(\mathbb{R})$, $f_{j,i} \not\equiv 0$, with $\mathbb{E}[f_{j,i}(X_i)] = 0$, and $\varepsilon_j \sim \mathcal{N}(0, \sigma_j^2)$ with $\sigma_j^2 > 0$ for $j = 1, \dots, p$. Likewise, we may write

$$X_j = \mu_j + \sum_{i \in \text{pa}_D^L(j)} \alpha_{j,i} X_i + \sum_{i \in \text{pa}_D^{\text{NL}}(j)} f_{j,i}(X_i) + \varepsilon_j,$$

with $\alpha_{j,i} \in \mathbb{R} \setminus \{0\}$, μ_j , $f_{j,i}$, ε_j as above, $\text{pa}_D^L(j) \cup \text{pa}_D^{\text{NL}}(j) = \text{pa}_D(j)$ and $\text{pa}_D^L(j) \cap \text{pa}_D^{\text{NL}}(j) = \emptyset$. Note that we do not *a priori* fix the sets $\text{pa}_D^L(j)$ and $\text{pa}_D^{\text{NL}}(j)$. For \mathbb{P} generated by a PLSEM with DAG D , the PLSEM corresponding to D is unique (Lemma A.2). Therefrom, we call an edge $i \rightarrow j$ in D a *(non-)linear edge*, if $f_{j,i}$ in the PLSEM corresponding to D is (non-)linear. Note that the concept of (non-)linearity of an edge is defined with respect to a specific DAG D . Depending on the orientations of other edges, the status of an edge $i \rightarrow j$ may change from linear to nonlinear. An example is given in Figure 1.



FIG 1. Two DAGs D_1 and D_2 with linear edges (dashed) and nonlinear edges (solid). Let us give a brief outlook: let \mathbb{P} be generated by a PLSEM with DAG D_1 . In this paper we prove that there exists a PLSEM with DAG D_2 that generates the same distribution \mathbb{P} . Moreover, we show that D_1 and D_2 are the only two DAGs with a corresponding PLSEM that generates \mathbb{P} . For now, simply note that $1 \rightarrow 3$ is linear in D_1 , but nonlinear in D_2 .

The restriction to additive SEMs is interesting from both a statistical and computational perspective as the estimation of additive functions is well understood and one largely avoids the curse of dimensionality. The assumption of

Gaussian noise is necessary for our theoretical results to hold. In fact, identifiability properties may deteriorate in partially linear models with arbitrary noise distributions, see Section 1.2.4. We therefore consider PLSEMs to be among the most general SEMs with reasonable estimation properties.

1.1.2. Main task: characterization of all PLSEMs that generate \mathbb{P}

The main task of this paper is the systematic characterization of all PLSEMs that generate a given distribution \mathbb{P} under very general assumptions. In particular: how do edge functions in different PLSEMs relate to each other? How does changing a single linear edge to a nonlinear edge affect the set of potential underlying PLSEMs? Do causal orderings of different DAGs corresponding to PLSEMs that generate \mathbb{P} share certain properties?

Under faithfulness, it may be natural to characterize all PLSEMs that generate \mathbb{P} by their corresponding DAGs as these DAGs are restricted to a subset of the Markov equivalence class (see Section 1.2.1). For a distribution \mathbb{P} that has been generated by a faithful PLSEM, we call the set of DAGs

$$\mathcal{D}(\mathbb{P}) := \left\{ D \mid \begin{array}{l} \mathbb{P} \text{ is faithful to } D \text{ and there exists a} \\ \text{PLSEM with DAG } D \text{ that generates } \mathbb{P} \end{array} \right\}$$

the (*PLSEM*) *distribution equivalence class*. Can we build on characterizations of the Markov equivalence class to characterize $\mathcal{D}(\mathbb{P})$? For example, can $\mathcal{D}(\mathbb{P})$ also be graphically represented by a single PDAG? Is it possible to efficiently estimate $\mathcal{D}(\mathbb{P})$? Before we explain our approaches to answer these questions in Section 1.3, let us briefly summarize related work.

1.2. Related work

First, in Section 1.2.1, we discuss the identifiability of general SEMs. We then motivate why our theoretical results close a relevant “gap” by reviewing existing identifiability results for two special cases of PLSEMs where either all the functions $f_{j,i}$ are linear (Section 1.2.2) or nonlinear (Section 1.2.3). Finally, we briefly comment on the assumption of Gaussian noise in Section 1.2.4.

1.2.1. Identifiability of general SEMs

In the general SEM as defined in equation (1.1) one cannot draw any conclusions about D given \mathbb{P} without making further assumptions. One such assumption commonly made is faithfulness (cf. Section 2.1). Under faithfulness, one can identify the Markov equivalence class of D (a set of DAGs that all entail the same conditional independences), see, for example, [15, Theorem 5.2.6]. Markov equivalence classes are well-characterized. In fact, the Markov equivalence class of a DAG D consists of all DAGs with the same skeleton and v-structures as D [26]

and can be graphically represented by a single partially directed graph (cf. Section 2.1). Moreover, any two Markov equivalent DAGs can be transformed into each other by a sequence of distinct covered edge reversals [6].

The estimation of the general SEM is difficult due to the curse of dimensionality in fully nonparametric estimation. In combination with the unidentifiability, this motivates the use of restricted SEMs, which have better estimation properties and for which it is possible to achieve (partial) identifiability of the SEM (even without assuming faithfulness), see Section 2.2 or [17] for an overview.

1.2.2. Special case of PLSEM: Linear Gaussian SEM

A widespread specification of PLSEMs are linear Gaussian SEMs, which have the same identifiability properties as the general SEMs: without additional assumptions they are unidentifiable, whereas under faithfulness, their distribution equivalence class equals the Markov equivalence class, see, for example, [21].

The estimation of the Markov equivalence class of linear Gaussian SEMs in the low-dimensional case has been addressed in e.g. [20, 5], whereas the high-dimensional scenario (requiring sparsity of the true underlying DAG) is discussed in e.g. [10, 25, 2, 13].

An exception of identifiability of linear Gaussian SEMs occurs if all ε_j have equal variances $\sigma_j^2 = \sigma^2 > 0, \forall j$. Under this assumption, the true underlying DAG D is identifiable [16]. Yet, the assumption of equal noise variances seems to be overly restrictive in many scenarios. In general, the linearity assumption may be rather restrictive if not implausible in some cases.

1.2.3. Special case of PLSEM: Nonlinear additive SEM with Gaussian noise

Interestingly, the assumption of exclusively nonlinear functions $f_{j,i}$ in equation (1.2) greatly improves the identifiability properties, see [9] for the bivariate case and [17] for a general treatment. In fact, if all $f_{j,i}$ are nonlinear and three times differentiable, $\mathcal{D}(\mathbb{P})$ only consists of the single true underlying DAG D [17, Corollary 31 (ii)]. The nonlinearity assumption is crucial, though. The authors provide an example where two DAGs are distribution equivalent if one of the nonlinear functions is replaced by a linear function [17, Example 26].

Various estimation methods have been introduced for additive nonlinear SEMs to infer the underlying DAG [17, 24, 14]. In particular, a restricted maximum likelihood estimation method called CAM, which is consistent in the low- and high-dimensional setting (assuming a sparse underlying DAG), has been proposed specifically for nonlinear additive SEMs with Gaussian noise [3].

1.2.4. The importance of Gaussian noise for the identifiability of PLSEMs

The identifiability properties of linear SEMs generally improve if one allows for non-Gaussian noise distributions. In fact, if all but one ε_j are assumed to

be non-Gaussian (commonly referred to as LiNGAM setting), the underlying DAG D is identifiable [19]. A general theory for linear SEMs with arbitrary noise distributions is presented in [8]. Both papers also propose estimation procedures for the respective model classes.

Unfortunately, the situation is different for PLSEMs: identifiability can be lost if one considers PLSEMs with non-Gaussian (or arbitrary) noise distributions. This can be seen from a specific example of a bivariate linear SEM with Gumbel-distributed noise, which is identifiable in the LiNGAM framework, but for which there exists a nonlinear additive backward model [9]. Still, this example seems to be rather particular. In fact, for bivariate additive SEMs, all unidentifiable cases of additive models can be classified into five categories, see [29, 17].

1.3. Our contribution

As discussed in Section 1.2, there exists a wide “identifiability gap” for PLSEMs. Their identifiability has only been studied for the two special cases of linear SEMs and entirely nonlinear additive SEMs. Moreover, to the best of our knowledge, it has not yet been understood to what extent (single) nonlinear functions in additive SEMs with Gaussian noise restrict the underlying causal model. We close the “identifiability gap” for PLSEMs and answer the questions raised in Section 1.1.2 with the following theoretical results:

- (A) A graphical representation of $\mathcal{D}(\mathbb{P})$ with a single partially directed graph $G_{\mathcal{D}(\mathbb{P})}$ in Section 2.1.1 (analogous to the use of CPDAGs to represent Markov equivalence classes).
- (B) A transformational characterization of $\mathcal{D}(\mathbb{P})$ through sequences of covered *linear* edge reversals in Section 2.1.2 (analogous to the characterization of Markov equivalence classes via sequences of covered edge reversals in [6]).
- (C) A functional characterization of PLSEMs in Section 2.2.1: all PLSEMs that generate the same distribution \mathbb{P} are constant rotations of each other.
- (D) A characterization of PLSEMs based on causal orderings in Section 2.2.2. In particular, it precisely specifies to what extent nonlinear functions in PLSEMs restrict the set of potential causal orderings.

The first two characterizations hold only under faithfulness, the third and fourth are general. We will give details on the precise interplay between nonlinearity and faithfulness in Section 2.3. Building on the transformational characterization result in (B) we provide an efficient score-based estimation procedure that outputs the graphical representation $G_{\mathcal{D}(\mathbb{P})}$ in (A) given \mathbb{P} and one DAG $D \in \mathcal{D}(\mathbb{P})$. The proposed algorithm only relies on sequences of local transformations and score computations and hence is feasible for large graphs with numbers of variables in the thousands (assuming reasonable sparsity). We demonstrate its performance on simulated data. Moreover, we derive its (high-dimensional) consistency based on the consistency proof of the CAM methodology in [3].

2. Comprehensive characterization of PLSEMs

This section contains our main theoretical results. They consist of characterizations of PLSEMs that generate a given distribution \mathbb{P} from various perspectives. In Section 2.1 we assume that \mathbb{P} is faithful to the underlying causal model and demonstrate that this leads to a transformational characterization and a graphical representation of $\mathcal{D}(\mathbb{P})$ very similar to the well-known counterparts characterizing a Markov equivalence class. Our main theoretical contributions, which hold under very general assumptions and, in particular, do not rely on the faithfulness assumption, are presented in Section 2.2. They fully characterize all PLSEMs that generate a given distribution \mathbb{P} on a functional level. Moreover, they explain how nonlinear functions impose very specific restrictions on the set of potential causal orderings. Section 2.3 brings together the two previous sections by discussing the precise interplay of nonlinearity and faithfulness.

2.1. Characterizations of $\mathcal{D}(\mathbb{P})$ under faithfulness

Let \mathbb{P} be generated by a PLSEM with DAG $D \in \mathcal{D}(\mathbb{P})$. The goal of this section is to characterize $\mathcal{D}(\mathbb{P})$. Recall that $\mathcal{D}(\mathbb{P})$ is the set of all DAGs D such that \mathbb{P} is faithful to D and there exists a PLSEM with DAG D that generates \mathbb{P} . In words, faithfulness means that no conditional independence relations other than those entailed by the Markov property hold, see e.g. [20]. In particular, it implies that $\mathcal{D}(\mathbb{P})$ is a subset of the Markov equivalence class and all DAGs in $\mathcal{D}(\mathbb{P})$ have the same skeleton and v -structures [26]. Markov equivalence classes can be graphically represented with single graphs, known as CPDAGs (also referred to as essential graphs, maximally oriented graphs or completed patterns) [6, 1, 12, 26], where an edge is directed if and only if it is oriented the same way in all the DAGs in the Markov equivalence class, else, it is undirected. The Markov equivalence class then equals the set of all DAGs that can be obtained from the CPDAG by orienting the undirected edges without creating new v -structures. In Section 2.1.1 we derive an analogous graphical representation of $\mathcal{D}(\mathbb{P})$.

Another useful (transformational) characterization result says that any two Markov equivalent DAGs can be transformed into each other by a sequence of distinct covered edge reversals [6]. We will demonstrate in Section 2.1.2 that a very similar principle transfers to $\mathcal{D}(\mathbb{P})$.

2.1.1. Graphical representation of $\mathcal{D}(\mathbb{P})$

The distribution equivalence class $\mathcal{D}(\mathbb{P})$ can be graphically represented by a single partially directed acyclic graph (PDAG). A PDAG is a graph with directed and undirected edges that does not contain any directed cycles. A *consistent DAG extension* of a PDAG is a DAG with the same skeleton, the same edge orientations on the directed subgraph of the PDAG, and no additional v -structures.

Definition 2.1. Let \mathcal{E} be a set of Markov equivalent DAGs. We denote by $G_{\mathcal{E}}$ the PDAG that has the same skeleton as the DAGs in \mathcal{E} and $i \rightarrow j$ in $G_{\mathcal{E}}$ if and only if $i \rightarrow j$ in all the DAGs in \mathcal{E} , else, $i - j$.

For a given distribution equivalence class $\mathcal{D}(\mathbb{P})$, the corresponding PDAG $G_{\mathcal{D}(\mathbb{P})}$ is uniquely defined by Definition 2.1. Moreover, $G_{\mathcal{D}(\mathbb{P})}$ is a graphical representation of $\mathcal{D}(\mathbb{P})$ in the following sense:

Theorem 2.1. $\mathcal{D}(\mathbb{P})$ equals the set of all consistent DAG extensions of $G_{\mathcal{D}(\mathbb{P})}$.

A proof can be found in Section A.1. Theorem 2.1 states that one can represent $\mathcal{D}(\mathbb{P})$ with a single PDAG $G_{\mathcal{D}(\mathbb{P})}$ without loss of information, as $\mathcal{D}(\mathbb{P})$ can be reconstructed from $G_{\mathcal{D}(\mathbb{P})}$ by listing all consistent DAG extensions. An example is given in Figure 2. Note that $G_{\mathcal{D}(\mathbb{P})}$ can be interpreted as a maximally oriented graph with respect to some background knowledge as defined in [12]. For details, we refer to Section 3.2.

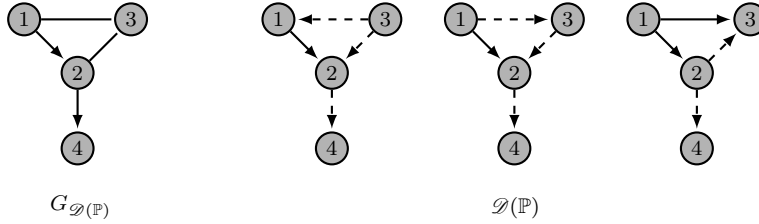


FIG 2. Graphical representation of $\mathcal{D}(\mathbb{P})$ with the single PDAG $G_{\mathcal{D}(\mathbb{P})}$. $\mathcal{D}(\mathbb{P})$ equals the set of all consistent DAG extensions of $G_{\mathcal{D}(\mathbb{P})}$. The graph with $2 \rightarrow 3 \rightarrow 1$ is not a consistent DAG extension of $G_{\mathcal{D}(\mathbb{P})}$ as it contains a cycle. Linear edges are dashed, nonlinear edges are solid.

Conceptually, this is completely analogous to the use of CPDAGs to represent Markov equivalence classes. There are important differences, though: first of all, necessary and sufficient conditions have been derived for a graph to be a CPDAG of a Markov equivalence class [1, Theorem 4.1]. These properties do not all transfer to $G_{\mathcal{D}(\mathbb{P})}$. For example, $G_{\mathcal{D}(\mathbb{P})}$ typically is not a chain graph, see Figure 2. Secondly, given a DAG D , the CPDAG (and hence a full characterization of the Markov equivalence class) can be obtained by an iterative application of three purely graphical orientation rules (R1-R3 in Figure 6) applied to the pattern of D [12]. This is not true for $G_{\mathcal{D}(\mathbb{P})}$ and $\mathcal{D}(\mathbb{P})$. It is still feasible to obtain $G_{\mathcal{D}(\mathbb{P})}$ from a DAG $D \in \mathcal{D}(\mathbb{P})$, but it is crucial to know which of the functions in the (unique) corresponding PLSEM (cf. Lemma A.2) are linear and which are nonlinear. We will show in Section 3 that the transformational characterization in Theorem 2.2 gives rise to a consistent and efficient score-based procedure to estimate $G_{\mathcal{D}(\mathbb{P})}$ based on $D \in \mathcal{D}(\mathbb{P})$ and samples of \mathbb{P} .

2.1.2. Transformational characterization of $\mathcal{D}(\mathbb{P})$

Given $D \in \mathcal{D}(\mathbb{P})$, the distribution equivalence class $\mathcal{D}(\mathbb{P})$ can be comprehensively characterized via sequences of local transformations of DAGs.

Theorem 2.2. Assume that \mathbb{P} has been generated by a PLSEM and that it is faithful to the underlying DAG. Then, the following two results hold:

- (a) Let $D \in \mathcal{D}(\mathbb{P})$, $i \rightarrow j$ covered in D , and D' be the DAG that differs from D only by the reversal of $i \rightarrow j$. Then, $D' \in \mathcal{D}(\mathbb{P})$ if and only if $i \rightarrow j$ is linear in D . Furthermore, if $i \rightarrow j$ is covered and nonlinear in D , then $i \rightarrow j$ in all DAGs in $\mathcal{D}(\mathbb{P})$.
- (b) Let $D, D' \in \mathcal{D}(\mathbb{P})$. Then there exists a sequence of distinct covered linear edge reversals that transforms D to D' .

A proof can be found in Section A.2 and an illustration is provided in Figure 3. Note that the interesting part of this result is that $\mathcal{D}(\mathbb{P})$ is connected with respect to covered linear edge reversals. It will be of particular importance in the design of score-based estimation procedures for $\mathcal{D}(\mathbb{P})$ and $G_{\mathcal{D}(\mathbb{P})}$ in Section 3.

Theorem 2.2 covers the two special cases discussed in Section 1.2: if all the functions $f_{j,i}$ in equation (1.2) are linear, $\mathcal{D}(\mathbb{P})$ (which, in this setting, is equal to the Markov equivalence class) can be fully characterized by sequences of covered edge reversals of D (as all the edges are linear). If, on the contrary, all the functions $f_{j,i}$ in equation (1.2) are nonlinear, $\mathcal{D}(\mathbb{P})$ only consists of the DAG D as there is no covered linear edge in D .

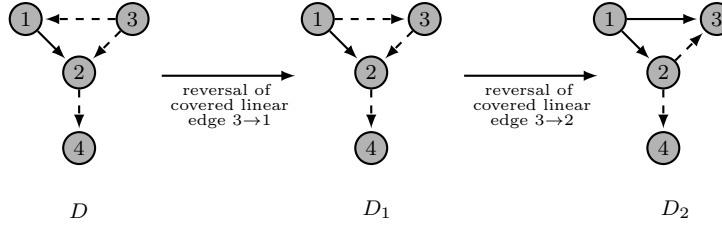


FIG 3. Transformational characterization of $\mathcal{D}(\mathbb{P})$ from Figure 2. Let $1 \rightarrow 2$ in D be nonlinear (solid) and all other edges in D be linear (dashed). Then, D_1 and D_2 can be reached from D by the displayed sequence of covered linear edge reversals. Note that in D and D_2 , $1 \rightarrow 2$ is covered but nonlinear and hence cannot be reversed by Theorem 2.2 (a). Moreover, $2 \rightarrow 4$ is not covered in any of D , D_1 and D_2 and hence cannot be reversed.

2.2. General characterizations not assuming faithfulness

In this section we give general characterizations of PLSEMs that generate the same distribution \mathbb{P} , both, from the perspective of causal orderings and from a functional viewpoint. The functional characterization in Section 2.2.1 describes how the $f_{j,i}$ of different PLSEMs relate to each other. The characterization via causal orderings in Section 2.2.2 describes the set of causal orderings, such that there exists a corresponding PLSEM that generates the given distribution \mathbb{P} . It will show that nonlinear functions impose a very specific structure on the model, which (perhaps surprisingly) is compatible with some of the previous theory on graphical models, as described in Section 1.2. Furthermore it will

help us understand in the general case how nonlinear functions restrict the set of PLSEMs that generate \mathbb{P} . Section 2.2.3 gives some intuition on the functional characterization in Section 2.2.1. Throughout this section, we assume that \mathbb{P} is generated by a PLSEM as defined in equation (1.2).

2.2.1. Functional characterization

Let us first characterize the result on the level of SEMs. Consider a PLSEM that generates \mathbb{P} ,

$$X_j = \mu_j + \sum_{i \in \text{pa}_D(j)} f_{j,i}(X_i) + \varepsilon_j,$$

where $f_{j,i}, D, \varepsilon_j, \mu_j, \sigma_j^2 = \text{Var}(\varepsilon_j)$ satisfy the assumptions from Section 1.1.1.

Let us define the function $F : \mathbb{R}^p \rightarrow \mathbb{R}^p$ by

$$F(x)_j := \frac{1}{\sigma_j} \left(x_j - \mu_j - \sum_{i \in \text{pa}_D(j)} f_{j,i}(x_i) \right). \quad (2.1)$$

It turns out to be convenient to work with this function F . Notably, we do not lose any information by working with F instead of $f_{j,i}, \text{pa}_D(j), \mu_j$ and σ_j as these quantities can be recovered from F . Specifically, we can easily obtain the distribution of the errors from the function F as

$$\sigma_j := 1/\partial_j F_j. \quad (2.2)$$

By definition, $F(X) \sim \mathcal{N}(0, \text{Id}_p)$. Hence, if $Z \sim \mathcal{N}(0, \text{Id}_p)$, then $F^{-1}(Z) \sim X$. Using this, we obtain $\mu_j = \mathbb{E}_Z[F^{-1}(Z)_j]$ and we can recover the functions $f_{j,i}$ from the function F using the equations

$$f'_{j,i} = -\sigma_j \partial_i F_j \quad \text{and} \quad \mathbb{E}_Z f_{j,i}(F^{-1}(Z)_i) = 0. \quad (2.3)$$

Note that the equation on the left hand side determines $f_{j,i}$ up to a constant, whereas the equation on the right hand side determines the constant using only quantities that can be calculated from F . In the same spirit, $\text{pa}_D(j)$ can be recovered from F via

$$\text{pa}_D(j) = \{i \neq j : \partial_i F_j \neq 0\}. \quad (2.4)$$

In this sense, instead of describing the PLSEM by $f_{j,i}, \text{pa}_D(j), \mu_j$ and σ_j it can simply be described by the function $F : \mathbb{R}^p \rightarrow \mathbb{R}^p$. Now let us define

$$\mathcal{F}(\mathbb{P}) := \{F : \mathbb{R}^p \mapsto \mathbb{R}^p : F \text{ suffices (2.1) for a PLSEM that generates } \mathbb{P}\}.$$

We call the functions in this set *PLSEM-functions*. Let us define the set of orthonormal matrices $\mathcal{O}_n(\mathbb{R}) = \{O \in \mathbb{R}^{n \times n} : OO^t = \text{Id}\}$. The following theorem follows from Theorem A.1, see Remark A.3 for details. It states that we can construct all PLSEMs that generate \mathbb{P} by essentially *rotating* F .

Theorem 2.3 (Characterization of potential PLSEMs). *For a given $F \in \mathcal{F}(\mathbb{P})$ there exists a set of (constant) rotations $\mathcal{O}_{\mathcal{F}(\mathbb{P})} \subset \mathcal{O}_n(\mathbb{R})$ such that*

$$\mathcal{F}(\mathbb{P}) = \{O \cdot F : O \in \mathcal{O}_{\mathcal{F}(\mathbb{P})}\}.$$

A description and explicit formulae for each $O \in \mathcal{O}_{\mathcal{F}(\mathbb{P})}$ can be found in the Appendix, Remark A.3.

Astonishingly, in this sense, all PLSEMs that generate \mathbb{P} are rotations of each other. The importance of this result lies in its simplicity: There are very simple linear relationships between the $f_{j,i}$ in one PLSEM and the $\hat{f}_{j,i}$ in another PLSEM. The formulae in the Appendix permit to fully characterize these matrices $\mathcal{O}_{\mathcal{F}(\mathbb{P})}$. In fact, the characterization in Theorem A.1 is the first step towards all other characterizations.

2.2.2. Characterization via causal orderings

This section discusses a characterization of all potential causal orderings of a given PLSEM. Let us define the set of *potential causal orderings* as

$$\mathcal{S}(\mathbb{P}) := \left\{ \sigma \text{ permutation on } \{1, \dots, p\} : \begin{array}{l} \text{there exists a PLSEM with DAG } D \\ \text{that generates } \mathbb{P} \text{ such that } \sigma(i) < \sigma(j) \text{ for all } i \rightarrow j \text{ in } D \end{array} \right\}.$$

Without assuming faithfulness, if all $f_{j,i}$ are linear, all permutations of $\{1, \dots, p\}$ are a causal ordering of a DAG corresponding to a PLSEM that generates \mathbb{P} . That is, $\mathcal{S}(\mathbb{P})$ is equal to the set of all permutations of $\{1, \dots, p\}$. Roughly, the more nonlinear functions in the PLSEM, the smaller the resulting set $\mathcal{S}(\mathbb{P})$. The interesting point is that nonlinear edges restrict $\mathcal{S}(\mathbb{P})$ in a very specific way. Before we state the theorem, consider a PLSEM that generates \mathbb{P} , define the function $F : \mathbb{R}^p \rightarrow \mathbb{R}^p$ as in equation (2.1) and define the set

$$\mathcal{V} := \{(i, j) \in \{1, \dots, p\}^2 : e_j^t (DF)^{-1} \partial_i^2 F \neq 0\}, \quad (2.5)$$

where e_j , $j = 1, \dots, p$ denotes the standard basis of \mathbb{R}^p and DF is the Jacobian of F . In some sense, we can think of $e_j^t (DF)^{-1} \partial_i^2 F \neq 0$ as “the effect from variable i to variable j is nonlinear”. We will discuss the set \mathcal{V} in more detail later. Then, the potential causal orderings can be characterized as follows:

Theorem 2.4 (Characterization of potential causal orderings).

$$\mathcal{S}(\mathbb{P}) = \{\sigma \text{ permutation on } \{1, \dots, p\} : \sigma(i) < \sigma(j) \text{ for all } (i, j) \in \mathcal{V}\}$$

The proof of this theorem can be found in Appendix A.4. In words, all permutations of the indices that do not swap any of the tuples in \mathcal{V} are a causal ordering of a DAG corresponding to a PLSEM that generates \mathbb{P} . And for all permutations of indices for which one of the tuples in \mathcal{V} is switched, there exists *no* PLSEM with this causal ordering that generates \mathbb{P} . Moreover, by Theorem A.2 (b), if $(i, j) \in \mathcal{V}$, then j is a descendant of i in every PLSEM that generates \mathbb{P} . Now let us give some intuition on the index tuples in the set \mathcal{V} .

Example 2.1. Consider the DAG $1 \rightarrow 2 \rightarrow 3$ and \mathbb{P} that has been generated by a PLSEM of the form $X_1 = \varepsilon_1, X_2 = f_{2,1}(X_1) + \varepsilon_2, X_3 = f_{3,2}(X_2) + \varepsilon_3$ with $\varepsilon \sim \mathcal{N}(0, \text{Id}_3)$.

- (a) Let $f_{2,1}(x) = 0.5x$ be linear, $f_{3,2}(x) = x^3$ be nonlinear. The corresponding PLSEM-function is $F(x) = (x_1, x_2 - 0.5x_1, x_3 - x_2^3)^t$. Using elementary calculations it can be seen that $e_j^t (DF)^{-1} \partial_i^2 F \neq 0$ only for $(i, j) = (2, 3)$. Hence, $\mathcal{V} = \{(2, 3)\}$ and all permutations σ respecting $\sigma(2) < \sigma(3)$ are a causal ordering of a DAG corresponding to a PLSEM that generates \mathbb{P} . For example, for the causal ordering $\sigma(2) < \sigma(3) < \sigma(1)$, there exists a (unique) PLSEM with DAG $1 \leftarrow 2 \rightarrow 3$ that generates \mathbb{P} .
- (b) Let $f_{2,1}(x) = x^3$ be nonlinear, $f_{3,2}(x) = 0.5x$ be linear. The corresponding PLSEM-function is $F(x) = (x_1, x_2 - x_1^3, x_3 - 0.5x_2)^t$. We obtain $\mathcal{V} = \{(1, 2), (1, 3)\}$ and all permutations σ with $\sigma(1) < \sigma(2)$ and $\sigma(1) < \sigma(3)$ are a causal ordering of a DAG corresponding to a PLSEM that generates \mathbb{P} . In particular, for $\sigma(1) < \sigma(3) < \sigma(2)$ we obtain that the PLSEM corresponding to the (unfaithful) DAG $1 \rightarrow 3 \rightarrow 2$ with $1 \rightarrow 2$ generates \mathbb{P} .

Let us make several concluding remarks: in (a), the causal ordering between nodes 1 and 3 is not fixed, whereas in (b), it is fixed. Hence, the set \mathcal{V} sometimes also fixes the causal ordering between two nodes that are not adjacent in the DAG corresponding to F . Secondly, in both examples, the causal ordering of nodes incident to nonlinear edges is fixed. This raises the question whether it is true in general that nonlinear edges cannot be reversed. The answer is no (see Figure 4), but in some sense, the models with “reversible nonlinear edges” are rather particular. Finally, if we make additional mild assumptions, stronger statements can be made about the index tuples in \mathcal{V} . We will discuss these issues further in Section 2.3.

2.2.3. Intuition on the functional characterization

This section motivates Theorem 2.3. Consider two functions $F, G \in \mathcal{F}(\mathbb{P})$ that correspond to two different PLSEMs. By Proposition A.1,

$$F(X) \sim \mathcal{N}(0, \text{Id}) \text{ and } G(X) \sim \mathcal{N}(0, \text{Id}). \quad (2.6)$$

Moreover, it follows from the definition of PLSEMs that F is invertible. Let $Z \sim \mathcal{N}(0, \text{Id}_p)$. Using equation (2.6) twice,

$$F^{-1}(Z) \sim X \text{ and } G(F^{-1}(Z)) \sim \mathcal{N}(0, \text{Id}).$$

Hence the function $J : \mathbb{R}^p \rightarrow \mathbb{R}^p$, $J := G(F^{-1})$ suffices $J(Z) \sim Z \sim \mathcal{N}(0, \text{Id})$. Furthermore, it can be shown that $|\det DJ| = 1$. Then, using the transformation formula, we obtain

$$\frac{1}{(2\pi)^{p/2}} \exp\left(-\frac{\|J(x)\|_2^2}{2}\right) = \frac{1}{(2\pi)^{p/2}} \exp\left(-\frac{\|x\|_2^2}{2}\right) \text{ for all } x \in \mathbb{R}^p.$$

By rearranging,

$$\|J(x)\|_2 = \|x\|_2 \text{ for all } x \in \mathbb{R}^p.$$

If we admit that J must be a linear function (which requires some work), this formula gives us $J \in \mathcal{O}_n(\mathbb{R}) := \{O \in \mathbb{R}^{p \times p} : OO^t = \text{Id}\}$ and it immediately follows that $G = JF$. This reasoning shows that the main work in proving Theorem 2.3 lies in showing that J is a linear function.

2.3. Understanding the interplay of nonlinearity and faithfulness

As indicated in Section 2.2.2, without further assumptions, some nonlinear edges can be reversed. An example is given in Figure 4. There, the edge $1 \rightarrow 3$ can be reversed even though $f_{3,1}$ is a nonlinear function in the PLSEM corresponding to D_1 . The issue here arises because the nonlinear effect from X_1 to X_3 in D_1 cancels out over two paths. If we write X_3 as a function of $\varepsilon_1, \varepsilon_2, \varepsilon_3$, that function is linear. The setting of D_1 in Figure 4 is rather particular as $\partial_1^2 f_{2,1}$ and $\partial_1^2 f_{3,1}$ are linearly dependent. As the function space $\mathcal{C}^2(\mathbb{R})$ is infinite dimensional, this is arguably a degenerate scenario. Note that faithfulness does not save us from this cancellation effect as \mathbb{P} is faithful to both, D_1 and D_2 .



FIG 4. Nonlinear edges can be reversed if nonlinear effects cancel out. $X_1 = \varepsilon_1$, $X_2 = X_1^2 + X_1 + \varepsilon_2$, $X_3 = X_2 - X_1^2 + \varepsilon_3$ with $\varepsilon \sim \mathcal{N}(0, \text{Id}_3)$ generates the same joint distribution of (X_1, X_2, X_3) as $X_3 = \tilde{\varepsilon}_3$, $X_1 = X_3/3 + \tilde{\varepsilon}_1$, $X_2 = X_1/2 + X_1^2 + X_3/2 + \tilde{\varepsilon}_2$ with $\tilde{\varepsilon}_3 \sim \mathcal{N}(0, 3)$, $\tilde{\varepsilon}_1 \sim \mathcal{N}(0, 2/3)$, $\tilde{\varepsilon}_2 \sim \mathcal{N}(0, 1/2)$ independent. This stems from the fact that the nonlinear parts of the functions $f_{2,1}(x)$ and $f_{3,1}(x)$ cancel out, i.e. $f_{2,1}'' + f_{3,1}'' = 0$. Note that this example does not contradict the previous theoretical results. It holds that $e_3^t (DF_1)^{-1} \partial_1^2 F \equiv 0$ for the PLSEM-function F corresponding to D_1 . Hence the causal ordering of D_2 does not contradict Theorem 2.4.

Nevertheless, we can rely on a different, rather weak assumption: consider a node i in a DAG D and assume that the corresponding functions in the set

$$\{\partial_i^2 f_{j',i} : j' \text{ is a child of } i \text{ in } D \text{ and } f_{j',i} \text{ is nonlinear}\}$$

are linearly independent. In other words: assume that the “nonlinear effects” from X_i on its children are linearly independent functions. Then these nonlinear edges cannot be reversed.

The following corollary is a direct implication of Theorem A.2 (a) and (b).

Corollary 2.1. *Consider a PLSEM and the corresponding distribution \mathbb{P} . Let j be a child of i in D and let $f_{j,i}$ be a nonlinear function. If the functions in the set $\{\partial_i^2 f_{j',i} : j' \text{ is a child of } i \text{ in } D \text{ and } f_{j',i} \text{ is nonlinear}\}$ are linearly independent, then j is a descendant of i in any other DAG D' of a PLSEM that generates \mathbb{P} .*

Intuitively, this should not be the end of the story: if an edge $i \rightarrow j$ is nonlinear, then usually there should also be a nonlinear relationship between i and the descendants of j . Hence it should be possible to infer some statements about the causal ordering of i and the descendants of j . In general, this is not true as demonstrated in Figure 5.



FIG 5. If \mathbb{P} is not faithful to D , descendants are not fixed. Node 4 is a descendant of node 1 in D_1 but not in D_2 . On the left hand side, $X_1 = \varepsilon_1$, $X_2 = X_1^2 + \varepsilon_2$, $X_3 = X_2 + \varepsilon_3$, $X_4 = X_3 - X_2 + \varepsilon_4$, with $\varepsilon \sim \mathcal{N}(0, \text{Id}_4)$. On the right hand side, $X_1 = \tilde{\varepsilon}_1$, $X_2 = X_1^2 + \tilde{\varepsilon}_2$, $X_3 = X_2 + 1/2 \cdot X_4 + \tilde{\varepsilon}_3$, $X_4 = \tilde{\varepsilon}_4$, where $\tilde{\varepsilon}_1 \sim \mathcal{N}(0, 1)$, $\tilde{\varepsilon}_2 \sim \mathcal{N}(0, 1)$, $\tilde{\varepsilon}_3 \sim \mathcal{N}(0, 1/2)$ and $\tilde{\varepsilon}_4 \sim \mathcal{N}(0, 2)$. Both PLSEMs generate the same distribution. Note that in this case, additional assumptions on the nonlinear function $f_{2,1}$ would not resolve the issue.

Under the assumption of faithfulness, additional statements can be made about descendants of j . In some sense the nonlinear effect from i on the descendants of j , mediated through some of the descendants of j , cannot “cancel out”. Hence, all descendants of j are fixed. The following corollary is a direct implication of Theorem A.2 (c) and (d).

Corollary 2.2. *Let the assumptions of Corollary 2.1 be true. In addition, let \mathbb{P} be faithful to the DAG D . Fix $k \neq i$. Then k is a descendant of i in each DAG D' of a PLSEM that generates \mathbb{P} if and only if k is a descendant of a nonlinear child of i in D .*

Note that we use the convention that a node is a descendant of itself. Corollary 2.2 guarantees that certain descendants of i are descendants of i in all DAGs D' of PLSEMs that generate \mathbb{P} . In that sense, it provides a simple criterion that tells us whether or not k is descendant of i in all of these DAGs. It is crucial to be precise: we do not assume that \mathbb{P} is faithful to D' , that means, we search over all PLSEMs that generate \mathbb{P} . If we search over the smaller space $\mathcal{D}(\mathbb{P})$, that is, additionally assume that \mathbb{P} is faithful to D' , the set of potential PLSEMs usually gets smaller. In many cases, there are some edges that are not fixed if we search over all PLSEMs, but fixed if we only search over PLSEMs with DAGs in $\mathcal{D}(\mathbb{P})$.

As discussed in Section 2.1.1, $\mathcal{D}(\mathbb{P})$ can be represented by a single PDAG $G_{\mathcal{D}(\mathbb{P})}$. In the following, we will discuss the estimation of $\mathcal{D}(\mathbb{P})$ and $G_{\mathcal{D}(\mathbb{P})}$.

3. Score-based estimation of $\mathcal{D}(\mathbb{P})$ and $G_{\mathcal{D}(\mathbb{P})}$

Consider \mathbb{P} that has been generated by a PLSEM and assume that \mathbb{P} is faithful to the underlying DAG. We denote by $\{X^{(i)}\}_{i=1,\dots,n}$ i.i.d. copies of $X \in \mathbb{R}^p$ and by \mathbb{P}_n their empirical distribution. The goal of this section is to derive a consistent score-based estimation procedure for the distribution equivalence class $\mathcal{D}(\mathbb{P})$ based on \mathbb{P}_n and one (true) DAG $D^0 \in \mathcal{D}(\mathbb{P})$. We first describe a “naive” recursive solution that lists all members of $\mathcal{D}(\mathbb{P})$ and motivate the score-based approach in Section 3.1. We then present a more efficient procedure that directly estimates the graphical representation $G_{\mathcal{D}(\mathbb{P})}$ as defined in Section 3.2. Both methods rely on the transformational characterization result in Theorem 2.2.

In practice, we may replace the true D^0 by an estimate, e.g., from the CAM methodology [3]. If the estimate is consistent for a DAG in $\mathcal{D}(\mathbb{P})$ we obtain consistency of our method for the entire distribution equivalence class $\mathcal{D}(\mathbb{P})$.

3.1. Estimation of $\mathcal{D}(\mathbb{P})$

Theorem 2.2 provides a straightforward way to list all members of $\mathcal{D}(\mathbb{P})$. Starting from the DAG D^0 , one can search over all sequences of distinct covered linear edges reversals. By Theorem 2.2 (a), all DAGs that are traversed are in $\mathcal{D}(\mathbb{P})$ and by Theorem 2.2 (b), $\mathcal{D}(\mathbb{P})$ is connected with respect to sequences of distinct covered linear edge reversals. Moreover, by Theorem 2.2 (a), an edge that is nonlinear and covered in a DAG in $\mathcal{D}(\mathbb{P})$ has the same orientation in all the members of $\mathcal{D}(\mathbb{P})$. These simple observations immediately lead to a recursive estimation procedure. Its population version is described in Algorithm 1. The inputs are D^0 (with all its edges marked as “unfixed”) and an oracle that answers the question if a specific edge in a DAG in $\mathcal{D}(\mathbb{P})$ is linear or nonlinear.

Algorithm 1 listAllDAGsPLSEM (population version)

```

1: if there is no covered edge in DAG  $D^0$  that is marked as unfixed then
2:   Add  $D^0$  to the distribution equivalence class  $\mathcal{D}(\mathbb{P})$  and terminate.
3: end if
4: Choose an covered edge  $i \rightarrow j$  in DAG  $D^0$  that is marked as unfixed.
5: if the edge  $i \rightarrow j$  is linear in  $D^0$  then
6:   Define a DAG  $D_1^0 := D^0$  with edge  $i \rightarrow j$  in  $D_1^0$  marked as fixed and a DAG  $D_2^0$  equal
   to  $D^0$  except for a reversed edge  $i \leftarrow j$  marked as fixed in  $D_2^0$ .
7:   Call the function listAllDAGsPLSEM recursively for both DAGs  $D_1^0$  and  $D_2^0$ .
8: else
9:   Mark the edge  $i \rightarrow j$  in  $D^0$  as fixed and call listAllDAGsPLSEM for DAG  $D^0$ .
10: end if

```

Unfortunately, the (true) information whether a selected covered edge $i \rightarrow j$ in a DAG $D \in \mathcal{D}(\mathbb{P})$ is linear or not is generally not available. Also, it cannot simply be deduced from the starting DAG D^0 as the status of the edge may have changed in D . For an example, see Figure 1: edge $1 \rightarrow 3$ is not covered and linear in D_1 but nonlinear and covered (and hence irreversible) in $D_2 \in \mathcal{D}(\mathbb{P})$.

To check the status of a covered edge in a given DAG $D \in \mathcal{D}(\mathbb{P})$, one could either test (non-)linearity of the functional component in the (unique) PLSEM

corresponding to D or rely on a score-based approach. In the following we are going to elaborate on the latter. We closely follow the approach presented in [3].

We assume that the functions $f_{j,i}$ in equation (1.2) are from a class of smooth functions $\mathcal{F}_i \subseteq \{f \in C^2(\mathbb{R}), \mathbb{E}[f(X_i)] = 0\}$, which is closed with respect to the $L_2(\mathbb{P}_{X_i})$ -norm and closed under linear transformations. For a set of given basis functions, we denote by $\mathcal{F}_{n,i} \subseteq \mathcal{F}_i$ the finite-dimensional approximation space which typically increases as n increases. The spaces of additive functions with components in \mathcal{F}_i and $\mathcal{F}_{n,i}$, respectively, are closed assuming an analogue of a minimal eigenvalue condition. All details are given in [3]. Without loss of generality, we assume $\mu_j = 0$ as in the original paper. For $D^0 \in \mathcal{D}(\mathbb{P})$, let $\theta^{D^0} := (\{f_{j,i}^{D^0}\}_{j=1,\dots,p, i \in \text{pa}_{D^0}(j)}, \{\sigma_j^{D^0}\}_{j=1,\dots,p})$ be the infinite-dimensional parameter of the corresponding PLSEM. The expected negative log-likelihood reads

$$\mathbb{E}[-\log p_{\theta^{D^0}}(X)] = \sum_{j=1}^p \log(\sigma_j^{D^0}) + C, \quad C = \frac{p}{2} \log(2\pi) + \frac{p}{2}.$$

All $D^0 \in \mathcal{D}(\mathbb{P})$ lead to the minimal expected negative log-likelihood, as by definition, the corresponding PLSEM generates the true distribution \mathbb{P} . For a misspecified model with wrong DAG $D \notin \mathcal{D}(\mathbb{P})$ we obtain the projected parameter $\theta^D = (\{f_{j,i}^D\}_{j=1,\dots,p, i \in \text{pa}_D(j)}, \{\sigma_j^D\}_{j=1,\dots,p})$ as

$$\begin{aligned} \{f_{j,i}^D\}_{i \in \text{pa}_D(j)} &= \underset{g_{j,i} \in \mathcal{F}_i}{\text{argmin}} \mathbb{E}[(X_j - \sum_{i \in \text{pa}_D(j)} g_{j,i}(X_i))^2] \\ (\sigma_j^D)^2 &= \mathbb{E}[(X_j - \sum_{i \in \text{pa}_D(j)} f_{j,i}^D(X_i))^2] \end{aligned}$$

with expected negative log-likelihood

$$\mathbb{E}[-\log(p_{\theta^D}^D(X))] = \sum_{j=1}^p \log(\sigma_j^D) + C, \quad C = \frac{p}{2} \log(2\pi) + \frac{p}{2},$$

where all expectations are taken with respect to the true distribution \mathbb{P} . We refer to $\mathbb{E}[-\log(p_{\theta^D}^D(X))]$ as the *score of D* and to $\log(\sigma_j^D)$ as *score of node j in D* . For a DAG $D^0 \in \mathcal{D}(\mathbb{P})$, let

$$\mathcal{C}(D^0) = \{D \mid D \text{ and } D^0 \text{ differ by a single covered nonlinear edge reversal}\}.$$

Then, for $D^0 \in \mathcal{D}(\mathbb{P})$ and $D \in \mathcal{C}(D^0)$ that (without loss of generality) only differ by the orientation of the covered edge between the nodes i and j , the difference in expected negative log-likelihood is given as

$$\begin{aligned} \mathbb{E}[-\log(p_{\theta^D}^D(X))] - \mathbb{E}[-\log(p_{\theta^{D^0}}^{D^0}(X))] \\ = \log(\sigma_i^D) + \log(\sigma_j^D) - \log(\sigma_i^{D^0}) - \log(\sigma_j^{D^0}). \end{aligned} \quad (3.1)$$

Since the score is decomposable over the nodes, the reversal of a covered edge only affects the scores locally at the two nodes i and j incident to the covered

edge. We denote by

$$\xi_p := \min_{\substack{D^0 \in \mathcal{D}(\mathbb{P}) \\ D \in \mathcal{C}(D^0)}} (\mathbb{E} [-\log(p_{\theta^D}^D(X))] - \mathbb{E} [-\log(p_{\theta^{D^0}}^{D^0}(X))]) \quad (3.2)$$

the *degree of separation* of true models in $\mathcal{D}(\mathbb{P})$ and misspecified models in $\mathcal{C}(\mathcal{D}(\mathbb{P}))$ that can be reached by the reversal of one covered nonlinear edge in any DAG $D^0 \in \mathcal{D}(\mathbb{P})$. From the transformational characterization in Theorem 2.2 it follows that $\xi_p > 0$. Combining equations (3.1) and (3.2) motivates the estimation procedure in Algorithm 2 that takes as inputs n samples $X^{(1)}, \dots, X^{(n)}$ and a DAG $D^0 \in \mathcal{D}(\mathbb{P})$ (with all its edges marked as “unfixed”) and outputs a score-based estimate $\hat{\mathcal{D}}_{n,p}$ of $\mathcal{D}(\mathbb{P})$.

Algorithm 2 listAllDAGsPLSEM

```

1: if there is no covered edge in DAG  $D^0$  that is marked as unfixed then
2:   Add  $D^0$  to  $\hat{\mathcal{D}}_{n,p}$  and terminate.
3: end if
4: Choose a covered edge  $i \rightarrow j$  in DAG  $D^0$  that is marked as unfixed. Denote by  $D'$  the
   DAG that equals  $D^0$  except for a reversed edge  $i \leftarrow j$ .
5: Additively regress  $X_i$  on  $X_{\text{pa}_{D^0}(i)}$ ,  $X_j$  on  $X_{\text{pa}_{D^0}(j)}$ ,  $X_i$  on  $X_{\text{pa}_{D^0}(i) \cup \{j\}}$ ,  $X_j$  on  $X_{\text{pa}_{D^0}(j)}$ 
6: Compute the standard deviations of the residuals to obtain  $\hat{\sigma}_i^{D^0}, \hat{\sigma}_j^{D^0}, \hat{\sigma}_i^{D'}, \hat{\sigma}_j^{D'}$ .
7: if  $|\log(\hat{\sigma}_i^{D'}) + \log(\hat{\sigma}_j^{D'}) - \log(\hat{\sigma}_i^{D^0}) - \log(\hat{\sigma}_j^{D^0})| < \alpha$  then
8:   Set  $D_1^0 := D^0$  with  $i \rightarrow j$  marked as fixed and  $D_2^0 := D'$  with  $i \leftarrow j$  marked as fixed.
9:   Call the function listAllDAGsPLSEM recursively for both DAGs  $D_1^0$  and  $D_2^0$ .
10: else
11:   Mark the edge  $i \rightarrow j$  in  $D^0$  as fixed and call listAllDAGsPLSEM for DAG  $D^0$ .
12: end if

```

To prove the (high-dimensional) consistency of the score-based estimation procedure, we make the following assumptions. For a function $h : \mathbb{R} \rightarrow \mathbb{R}$, we write $P(h) = \mathbb{E}[h(X)]$ and $P_n(h) = \frac{1}{n} \sum_{i=1}^n h(X^{(i)})$.

Assumption 3.1.

(i) *Uniform upper bound on node degrees:*

$$\max_{\substack{D \in \mathcal{D}(\mathbb{P}) \cup \mathcal{C}(\mathcal{D}(\mathbb{P})) \\ j=1, \dots, p}} \deg_D(j) \leq M \text{ for some positive constant } M < \infty.$$

(ii) *Uniform lower bound on error variances:*

$$\min_{\substack{D \in \mathcal{D}(\mathbb{P}) \cup \mathcal{C}(\mathcal{D}(\mathbb{P})) \\ j=1, \dots, p}} (\sigma_j^D)^2 \geq L > 0.$$

(iii) *Empirical process bound:*

$$\max_{\substack{D \in \mathcal{D}(\mathbb{P}) \cup \mathcal{C}(\mathcal{D}(\mathbb{P})) \\ j=1, \dots, p}} \Delta_{n,j}^D = o_P(1),$$

$$\text{where } \Delta_{n,j}^D = \sup_{g_{j,i} \in \mathcal{F}_i} |(P_n - P)((X_j - \sum_{i \in \text{pa}_D(j)} g_{j,i}(X_i))^2)|.$$

(iv) *Control of approximation error:*

$$\max_{\substack{D^0 \in \mathcal{D}(\mathbb{P}) \\ j=1, \dots, p}} |\gamma_{n,j}^{D^0}| = o(1),$$

where

$$\gamma_{n,j}^{D^0} = \mathbb{E}[(X_j - \sum_{i \in \text{pa}_{D^0}(j)} f_{n;j,i}^{D^0}(X_i))^2] - \mathbb{E}[(X_j - \sum_{i \in \text{pa}_{D^0}(j)} f_{j,i}^{D^0}(X_i))^2]$$

with

$$f_{n;j,i}^{D^0} = \underset{g_{j,i} \in \mathcal{F}_{n,i}}{\text{argmin}} \mathbb{E}[(X_j - \sum_{i \in \text{pa}_{D^0}(j)} g_{j,i}(X_i))^2]$$

and $\mathcal{F}_{n,i}$ are the approximation spaces as introduced before.

Assumption 3.1 (i) is satisfied if D^0 has bounded node degrees, as all DAGs under consideration are restricted to the same skeleton and hence all have equal node degrees. In the low-dimensional setting, Assumption 3.1 (iii) is justified by [3, Lemma 5] under the assumptions mentioned there. In the high-dimensional setting, it follows from [3, Lemma 6] and $\sqrt{\log(p)}/n = o(1)$ together with Assumption 3.1 (i) and the assumptions mentioned in the original paper. Assumption 3.1 (iv) can be ensured by requiring a smoothness condition on the coefficients of the basis expansion for the true functions [3, Section 4.2]. A proof of Theorem 3.1 can be found in Section A.6.1.

Theorem 3.1. *Under Assumption 3.1 and $\xi_p \geq \xi_0 > 0$, for any $\alpha \in (0, \xi_0)$,*

$$\mathbb{P}[\widehat{\mathcal{D}}_{n,p} = \mathcal{D}(\mathbb{P})] \rightarrow 1 \quad (n \rightarrow \infty)$$

Remark 3.1. *The assumption on the degree of separation of true and wrong models in [3] is stricter and would imply the uniform bound $\xi_p/p \geq \xi_0 > 0$, whereas here we only require $\xi_p \geq \xi_0 > 0$. As we are given a true DAG $D^0 \in \mathcal{D}(\mathbb{P})$, we solely perform local transformations of DAGs thanks to the transformational characterization result in Theorem 2.2. This only affects the scores of two nodes and allows us to rely on this much weaker gap condition.*

3.2. Estimation of $G_{\mathcal{D}(\mathbb{P})}$

The estimation of all DAGs in $\mathcal{D}(\mathbb{P})$ is feasible but may be computationally intractable in the presence of many linear edges. For example, if D^0 is a fully connected DAG with p nodes and all its edges are linear, the number of DAGs in $\mathcal{D}(\mathbb{P})$ corresponds to the number of causal orderings of p nodes which is $p!$. It therefore would be desirable to have a procedure that works without enumerating all DAGs in $\mathcal{D}(\mathbb{P})$. In this section we are going to describe such a procedure that directly estimates the maximally oriented PDAG $G_{\mathcal{D}(\mathbb{P})}$ defined in Section 2.1.1. Recall that by Theorem 2.1, this fully characterizes $\mathcal{D}(\mathbb{P})$, as $\mathcal{D}(\mathbb{P})$ can be recovered from $G_{\mathcal{D}(\mathbb{P})}$ by listing all consistent DAG extensions.

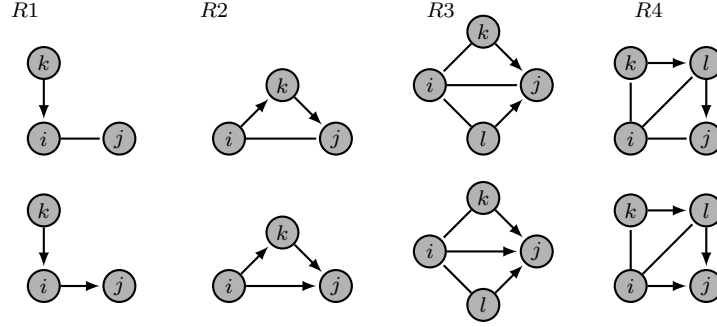


FIG 6. Orientation rules $R1$ - $R4$ for Markov equivalence classes with background knowledge from [12]. If there is an edge constellation as in the top row, $i - j$ is oriented as $i \rightarrow j$ when closing orientations under $R1$ - $R4$.

The main idea is the following: instead of traversing the space of DAGs, we traverse the space of maximally oriented PDAGs that represent sets of distribution equivalent DAGs. As an example, let $D^0 \in \mathcal{D}(\mathbb{P})$ and $i \rightarrow j$ be covered and linear in D^0 . By Theorem 2.2 (a), the DAG D' that only differs from D^0 by the reversal of $i \rightarrow j$ is in $\mathcal{D}(\mathbb{P})$. Instead of memorizing both, D^0 and D' , and recursively searching over sequences of covered linear edge reversals from both of these DAGs as in Algorithms 1 and 2, we represent D^0 and D' by the PDAG G that is maximally oriented with respect to the set of DAGs $\{D^0, D'\}$. By Definition 2.1, G equals D^0 but for an undirected edge $i - j$. To construct $G_{\mathcal{D}(\mathbb{P})}$, the idea is now to iteratively modify G by either fixing or removing orientations of directed edges if they are nonlinear or linear in one of the consistent DAG extensions of G in which they are covered. For that to work based on G only, that is, without listing all consistent DAG extensions of G , the two key questions are the following:

- (Q1) For $i \rightarrow j$ in a maximally oriented PDAG G , can we decide based on G only if there is a consistent DAG extension of G in which $i \rightarrow j$ is covered?
- (Q2) If $i \rightarrow j$ is known to be covered in a consistent DAG extension of G : can we derive a score-based check if $i \rightarrow j$ is linear or nonlinear in this extension based on G ?

Interestingly, the answer to both questions is yes (cf. Lemma 3.1) and can be derived from a related theory on how background knowledge on specific edge orientations restricts the Markov equivalence class. It was shown in [12, Theorems 2 & 4] that for a pattern P of a DAG, consistent background knowledge \mathcal{K} (in our case: additional knowledge on edge orientations due to nonlinear functions in the PLSEM) can be incorporated by simply orienting these edges in P and closing orientations under a set of four sound and complete graphical orientation rules $R1$ - $R4$, which are depicted in Figure 6. The resulting PDAG, which we denote by $G_{P, \mathcal{K}}$, is maximally oriented with respect to the set of all Markov equivalent DAGs with edge orientations that comply with the back-

ground knowledge.

It is important to note that we generally do not obtain $G_{\mathcal{D}(\mathbb{P})}$ if we simply add all nonlinear edges in D^0 as background knowledge \mathcal{K} and close orientations under R1-R4. The resulting maximally oriented PDAG $G_{P,\mathcal{K}}$ is typically not equal to $G_{\mathcal{D}(\mathbb{P})}$. For an example, consider D_1 in Figure 1 and denote by P_1 its pattern. For $\mathcal{K} = \{1 \rightarrow 2\}$ we obtain the PDAG $G_{P_1,\mathcal{K}}$ with undirected edge $1 - 3$. But $1 \rightarrow 3$ in $G_{\mathcal{D}(\mathbb{P})}$ by Definition 2.1 as $\mathcal{D}(\mathbb{P}) = \{D_1, D_2\}$. This illustrates that we have to add all edges to \mathcal{K} that are nonlinear in a DAG in $\mathcal{D}(\mathbb{P})$ in which they are covered ($1 \rightarrow 3$ is covered and nonlinear in D_2).

Lemma 3.1. *Let P be the pattern of a DAG and \mathcal{K} a consistent set of background knowledge (not containing directed edges of P). Let $G_{P,\mathcal{K}}$ denote the maximally oriented graph with respect to P and \mathcal{K} with orientations closed under R1-R4.*

- (a) *Edge $i \rightarrow j$ in \mathcal{K} is not covered in any of the consistent DAG extensions of $G_{P,\mathcal{K}}$ if and only if $G_{P,\mathcal{K}} = G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}$.*
- (b) *If $G_{P,\mathcal{K}} \neq G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}$, there exists a consistent DAG extension of $G_{P,\mathcal{K}}$ in which $\text{pa}_{G_{P,\mathcal{K}}}(j) \setminus \{i\}$ is a cover for $i \rightarrow j$.*

A proof is given in Section A.6.2. By construction, $G_{P,\mathcal{K}} = G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}$ if and only if the orientation of $i \rightarrow j$ in $G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}$ is implied by one of R1-R4 applied to $G_{P,\mathcal{K}}$ with undirected edge $i - j$. Hence, Lemma 3.1 (a) answers (Q1) as it provides a simple graphical criterion to check whether $i \rightarrow j$ in $G_{P,\mathcal{K}}$ is covered in one of the consistent DAG extensions of $G_{P,\mathcal{K}}$ based on $G_{P,\mathcal{K}}$ only. Note that part (a) is closely related to [1, Section 5], where the authors construct the CPDAG (representing the Markov equivalence class) from a given DAG by removing edge orientations that are not implied by a set of graphical orientation rules, which contain R1-R3 in Figure 6. Lemma 3.1 (b) answers (Q2): it allows us to implement a score-based check whether $i \rightarrow j$ is linear or nonlinear in a DAG extension of $G_{P,\mathcal{K}}$ in which it is covered by simply reading off the parents of j in $G_{P,\mathcal{K}}$ and use them as a cover for $i \rightarrow j$. Details are given in Remark 3.2.

We now propose the following iterative estimation procedure for $G_{\mathcal{D}(\mathbb{P})}$: let $D^0 \in \mathcal{D}(\mathbb{P})$ be given, P denote its pattern and define $\mathcal{K}_1 := \mathcal{K}_1^{\text{init}} \cup \mathcal{K}_1^{\text{nonl}}$, where $\mathcal{K}_1^{\text{init}}$ contains all directed edges in D^0 that are undirected in P and $\mathcal{K}_1^{\text{nonl}} := \emptyset$. By construction, $G_{P,\mathcal{K}_1} = D^0$. For $k \geq 1$, in each iteration k to $k+1$, we apply Lemma 3.1 (a) and use R1-R4 to select an edge $\{i \rightarrow j\} \in \mathcal{K}_k^{\text{init}}$ ($i \rightarrow j$ in G_{P,\mathcal{K}_k}) that is covered in a consistent DAG extension of G_{P,\mathcal{K}_k} (that is, not implied by any of R1-R4). If $\mathcal{K}_k^{\text{init}} = \emptyset$ or no such edge exists, we stop and output G_{P,\mathcal{K}_k} . Else, we check whether $i \rightarrow j$ is linear or nonlinear in a consistent DAG extension in which it is covered and construct a new set of background knowledge $\mathcal{K}_{k+1} := \mathcal{K}_{k+1}^{\text{init}} \cup \mathcal{K}_{k+1}^{\text{nonl}} \subseteq \mathcal{K}_k$ according to the following rules:

Case 1: If $i \rightarrow j$ is linear, $\mathcal{K}_{k+1}^{\text{nonl}} = \mathcal{K}_k^{\text{nonl}}$ and $\mathcal{K}_{k+1}^{\text{init}} = \mathcal{K}_k^{\text{init}} \setminus \{i \rightarrow j\}$.
Case 2: If $i \rightarrow j$ is nonlinear, $\mathcal{K}_{k+1}^{\text{nonl}} = \mathcal{K}_k^{\text{nonl}} \cup \{i \rightarrow j\}$ and $\mathcal{K}_{k+1}^{\text{init}} = \mathcal{K}_k^{\text{init}} \setminus \{i \rightarrow j\}$.

In particular, by construction, Case 1 implies that $i - j$ in all G_{P,\mathcal{K}_l} for $l > k$, whereas Case 2 fixes the orientation $i \rightarrow j$ in all G_{P,\mathcal{K}_l} for $l > k$.

Lemma 3.2. *Let $\{\mathcal{K}_k\}_k$ be constructed as described above. Then, the corresponding sequence of maximally oriented PDAGs $\{G_{P, \mathcal{K}_k}\}_k$ converges to $G_{\mathcal{D}(\mathbb{P})}$.*

A proof is given in Section A.6.3 and an illustration is provided in Figure 7. As in both cases, $|\mathcal{K}_{k+1}^{\text{init}}| = |\mathcal{K}_k^{\text{init}}| - 1$, $\{G_{P, \mathcal{K}_k}\}_k$ converges to $G_{\mathcal{D}(\mathbb{P})}$ after at most $|\mathcal{K}_1^{\text{init}}|$ iterations, where $|\mathcal{K}_1^{\text{init}}|$ is the number of undirected edges in P .

Remark 3.2. *Let $\{i \rightarrow j\} \in \mathcal{K}_k^{\text{init}}$ be the edge chosen in iteration k to $k+1$. By Lemma 3.1 (b), $S := \text{pa}_{G_{P, \mathcal{K}_k}}(j) \setminus \{i\}$ is a cover of $i \rightarrow j$ in one of the consistent DAG extensions of G_{P, \mathcal{K}_k} . From that, we easily obtain a score-based version: we simply regress X_i on X_S and X_j on $X_{S \cup \{i\}}$ to obtain the estimates $\hat{\sigma}_i, \hat{\sigma}_j$ of the standard deviations of the residuals at nodes i and j for $i \rightarrow j$. Similarly, we regress X_i on $X_{S \cup \{j\}}$ and X_j on X_S to get $\hat{\sigma}'_i, \hat{\sigma}'_j$ for $i \leftarrow j$. If the estimated score difference $|\log(\hat{\sigma}'_i) + \log(\hat{\sigma}'_j) - \log(\hat{\sigma}_i) - \log(\hat{\sigma}_j)|$ is smaller than α , we conclude that $i \rightarrow j$ is linear, else, nonlinear. The pseudo-code of the score-based procedure is provided in Algorithm 3. It outputs an estimate $\hat{G}_{n,p}$ of $G_{\mathcal{D}(\mathbb{P})}$ based on n samples $X^{(1)}, \dots, X^{(n)}$ and $D^0 \in \mathcal{D}(\mathbb{P})$.*

Algorithm 3 computeGDPX

```

1: Initialize  $\hat{G}_{n,p} \leftarrow D^0$ ,  $k \leftarrow 1$ ,  $\mathcal{K}_1^{\text{init}} \leftarrow \emptyset$  and  $\mathcal{K}_1^{\text{nonl}} \leftarrow \emptyset$ .
2: Construct the pattern  $P$  of  $D^0$ .
3: Add directed edges in  $D^0$  that are undirected in  $P$  to  $\mathcal{K}_1^{\text{init}}$ .
4: while There is  $i \rightarrow j$  in  $\mathcal{K}_k^{\text{init}}$ , such that its orientation is not implied by applying rules
   R1, R2, R3 or R4 to  $\hat{G}_{n,p}$  with undirected edge  $i - j$  do
5:   Use  $\text{pa}_{\hat{G}_{n,p}}(j) \setminus \{i\}$  to cover  $i \rightarrow j$  and estimate the standard deviations  $\hat{\sigma}_i, \hat{\sigma}_j, \hat{\sigma}'_i$  and
    $\hat{\sigma}'_j$  of the residuals as described in Remark 3.2.
6:   if  $|\log(\hat{\sigma}'_i) + \log(\hat{\sigma}'_j) - \log(\hat{\sigma}_i) - \log(\hat{\sigma}_j)| < \alpha$  then
7:     Set  $\mathcal{K}_{k+1}^{\text{init}} \leftarrow \mathcal{K}_k^{\text{init}} \setminus \{i \rightarrow j\}$  and replace  $i \rightarrow j$  by  $i - j$  in  $\hat{G}_{n,p}$ .
8:   else
9:     Set  $\mathcal{K}_{k+1}^{\text{init}} \leftarrow \mathcal{K}_k^{\text{init}} \setminus \{i \rightarrow j\}$  and keep  $i \rightarrow j$  in  $\hat{G}_{n,p}$ .
10:  end if
11:   $k \leftarrow k + 1$ .
12: end while
13: return Estimated PDAG  $\hat{G}_{n,p}$  representing  $\mathcal{D}(\mathbb{P})$ .

```

A major advantage of Algorithm 3 is that it can be implemented based on one adjacency matrix only that is updated in every iteration.

Theorem 3.2. *Under Assumption 3.1 and $\xi_p \geq \xi_0 > 0$, for any $\alpha \in (0, \xi_0)$,*

$$\mathbb{P} \left[\hat{G}_{n,p} = G_{\mathcal{D}(\mathbb{P})} \right] \rightarrow 1 \quad (n \rightarrow \infty)$$

Proof. The correctness of Algorithm 3 is proved in Lemma 3.2. The consistency of the score-based estimation follows from the proof of Theorem 3.1. \square

4. Simulations

In this section we empirically analyze the performance of `computeGDPX` (Algorithm 3) in various settings. Consider \mathbb{P} that has been generated by a faithful

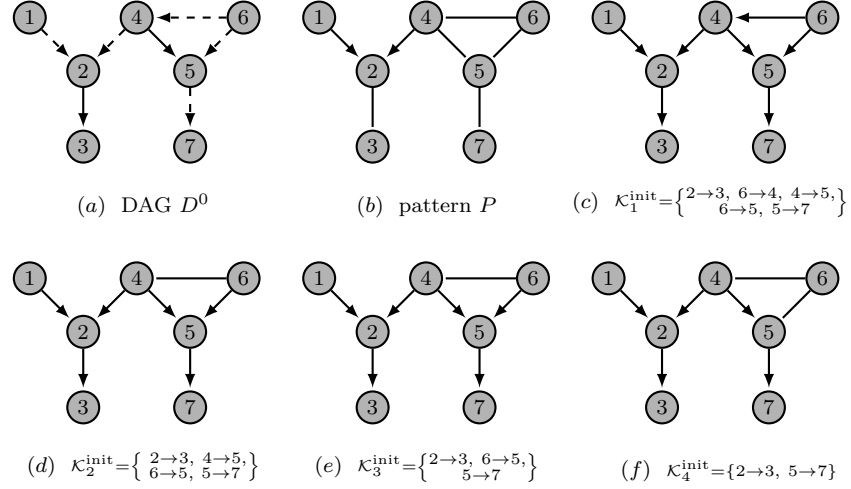


FIG 7. Illustration of Algorithm 3. (a) DAG D^0 with linear edges (dashed) and nonlinear edges (solid). (b) step 2: pattern P of D^0 . (c) step 3: directed edges in D^0 that are undirected in P are added to $\mathcal{K}_1^{\text{init}}$. By construction, $\hat{G}_{n,p} = D^0$. (c)-(f) steps 4-12: $4 \leftarrow 6$ is covered and linear in (c), hence, orientation is removed in $\hat{G}_{n,p}$ in (d). $4 \rightarrow 5$ is covered and nonlinear in (d), hence, orientation is fixed in $\hat{G}_{n,p}$ in (e). $6 \rightarrow 5$ is covered and linear in a consistent DAG extension of (e), hence, orientation is removed in $\hat{G}_{n,p}$ in (f). As both edges in $\mathcal{K}_4^{\text{init}}$ are implied by R1 in (f), they are not covered in any of the consistent DAG extensions of $\hat{G}_{n,p}$ in (f). Concludingly, $\hat{G}_{n,p} = G_{\mathcal{D}(\mathbb{P})}$ in (f).

PLSEM with known DAG D^0 . The goal is to estimate the corresponding distribution equivalence class $\mathcal{D}(\mathbb{P})$ based on D^0 and samples of \mathbb{P} . In Section 4.1, we start with a description of the simulation setting. We then briefly comment on a population version of Algorithm 3 in Section 4.2, which is used to obtain the underlying true distribution equivalence class $\mathcal{D}(\mathbb{P})$. In the subsequent sections we examine the role of the tuning parameter α (Section 4.3), the performance in low- and high-dimensional settings (Section 4.4) and the computation time (Section 4.5).

4.1. Simulation setting and implementation details

Throughout the section, let p denote the number of variables, n the number of samples, n_{rep} the number of repetitions of an experiment, p_c the probability to connect two nodes by an edge and p_{lin} the probability that an edge is linear. For each experiment we generate n_{rep} random true DAGs D^0 with the function `randomDAG` in the R-package `pcalg` [11] with parameters $\mathbf{n} = p$ and `prob` = p_c . For each of the random DAGs, we generate n samples of \mathbb{P} from a PLSEM with edge functions chosen as follows: with probability p_{lin} , $f_{j,i}(x) = \alpha_{j,i} \cdot x$ is linear with $\alpha_{j,i}$ randomly drawn from $[-1.5, -0.5] \cup [0.5, 1.5]$. Otherwise, $f_{j,i}(x)$ is nonlinear and randomly drawn from the set $\{c_0 \cdot \cos(c_1 \cdot (x - c_2)), c_0 \cdot$

$\tanh(c_1 \cdot (x - c_2))$ to have a mix of monotone and non-monotone functions in the PLSEM. In order to be able to empirically support our theoretical findings we choose the parameters $c_0 \sim \text{Unif}([-2, -1] \cup [1, 2])$, $c_1 \sim \text{Unif}([1, 2])$ and $c_2 \sim \text{Unif}([- \pi/3, \pi/3])$ such that the nonlinear functions are “sufficiently nonlinear” and not too close to linear functions. Exemplary randomly generated nonlinear functions are shown in Figure 8. The noise variables satisfy $\varepsilon_j \sim \mathcal{N}(0, \sigma_j^2)$ with $\sigma_j^2 \sim \text{Unif}([1, 2])$ for source nodes (nodes with empty parental set) and $\sigma_j^2 \sim \text{Unif}([1/4, 1/2])$ otherwise.

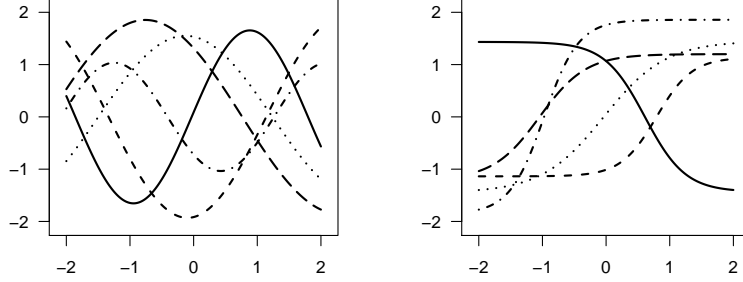


FIG 8. Exemplary nonlinear functions used in simulated PLSEMs.

In order to estimate the residuals in step 5 of `computeGDPX`, we use additive model fitting based on the R-package `mgcv` with default settings [27, 28]. The basis dimension for each smooth term is set to 6.

There exists no state-of-the-art method that we can compare our algorithm with. In principle, given D^0 , we can estimate the corresponding PLSEMs for all DAGs in the Markov equivalence class of D^0 and compute their scores. This also gives us an estimate for $\mathcal{D}(\mathbb{P})$, but as explained in Section 3.2, is less efficient than `computeGDPX`. We therefore only evaluate how accurately `computeGDPX` estimates $G_{\mathcal{D}(\mathbb{P})}$. For that, let $G_{\mathcal{D}(\mathbb{P})}$ and \hat{G} denote the true and estimated graphical representations of $\mathcal{D}(\mathbb{P})$, respectively. We count (i) the number of edges that are undirected in $G_{\mathcal{D}(\mathbb{P})}$ but directed in \hat{G} (“falsely kept orientations”) and (ii) the number of edges that are directed in $G_{\mathcal{D}(\mathbb{P})}$ but undirected in \hat{G} (“falsely removed orientations”). Note that as we assume faithfulness, all DAGs in $\mathcal{D}(\mathbb{P})$ have the same CPDAG. By construction, `computeGDPX` does not falsely remove orientations on the directed part of the CPDAG as all these edges are not covered in any of the consistent DAG extensions. To obtain the percentages shown in Figures 9 to 11 we therefore only divide by the number of undirected edges in the CPDAG. The percentages then reflect a measure for the fraction of “correct score-based decisions”.

4.2. Reference method for true distribution equivalence class $\mathcal{D}(\mathbb{P})$

To be able to characterize the true distribution equivalence class based on D^0 and the corresponding PLSEM we assume that for each $i \in \{1, \dots, p\}$, the functions in the set $\{\partial_i^2 f_{j,i} : j \text{ is a child of } i \text{ in } D^0 \text{ and } f_{j,i} \text{ is nonlinear}\}_i$ are linearly

independent for the PLSEM with DAG D^0 that generates \mathbb{P} . As all functions in our simulations are randomly drawn (cf. Section 4.1), the assumption is satisfied with probability one for D^0 and the corresponding edge functions.

This additional assumption rules out cases where nonlinear effects in D^0 exactly cancel out over different paths and hence excludes cases as in Figure 4 where nonlinear edges may be reversed. In particular, it allows us to use Theorem A.2 to obtain $G_{\mathcal{D}(\mathbb{P})}$ only based on D^0 and knowledge of the functions in the corresponding PLSEM: first, we use Theorem A.2 (c) to construct the set \mathcal{V} . For all nodes i in D^0 , corresponding sets of nonlinear children C_i (as defined in Section A.5) and $k \neq i$, we add (i, k) to \mathcal{V} if k is a descendant of a node in C_i . In principle, we now apply Algorithm 3, but instead of the score-based decision in steps 6-9, we use the set \mathcal{V} to decide about edge orientations. Let $i \rightarrow j$ be the edge chosen in step 4 and D one of the consistent DAG extensions in which $i \rightarrow j$ is covered. If $(i, j) \in \mathcal{V}$, by Theorem A.2 (d) and Remark A.5, $i \rightarrow j$ in all DAGs of a PLSEM that generates \mathbb{P} . Hence, in particular, $i \rightarrow j$ in all DAGs in $\mathcal{D}(\mathbb{P})$ and by definition, $i \rightarrow j$ in $G_{\mathcal{D}(\mathbb{P})}$. If $(i, j) \notin \mathcal{V}$, by Lemma A.1, the DAG D' that differs from D only by reversing $i \rightarrow j$ is in $\mathcal{D}(\mathbb{P})$. Hence, by definition, $i - j$ in $G_{\mathcal{D}(\mathbb{P})}$.

4.3. The role of α for varying sample size

In `computeGDPX`, the score-based decision whether a selected covered edge is linear or nonlinear is based on a comparison of the absolute difference of the expected negative log-likelihood scores of two models with a parameter α . Optimally, one would choose α close to ξ_p , see equation (3.2), but ξ_p depends on the setting (number of variables, sparsity of the DAG, degree of nonlinearity of the nonlinear functions, etc.) and is unknown. In practice, the parameter α reflects a measure of how conservative the estimate \hat{G} of $G_{\mathcal{D}(\mathbb{P})}$ is (in the sense of how many causal statements can be made). For example, choosing α large results in a conservative estimate \hat{G} with many undirected edges (a large set $\mathcal{D}(\mathbb{P})$ of equivalent DAGs). In Figures 9 and 10, we empirically analyze the dependence of \hat{G} on α for different sample sizes for sparse and dense graphs, respectively.

`computeGDPX` exhibits a good performance for a wide range of values of α . In particular, as the sample size increases, choosing α small results in very accurate estimates \hat{G} of $G_{\mathcal{D}(\mathbb{P})}$. The sparsity of the DAG does not strongly influence the results.

4.4. The dependence on p : low- and high-dimensional setting

From the fact that `computeGDPX` only relies on local score computations, we expect that its performance does not strongly depend on the number of variables p as long as the neighborhood sizes in the DAGs (the node degrees) are similar for different values of p . We simulate $n_{\text{rep}} = 100$ random DAGs with $p = 10$, $p = 100$ and $p = 1000$ nodes, respectively. Moreover, we set $p_c = 2/(p-1)$ which results in an expected number of p edges and an expected node degree of 2 for

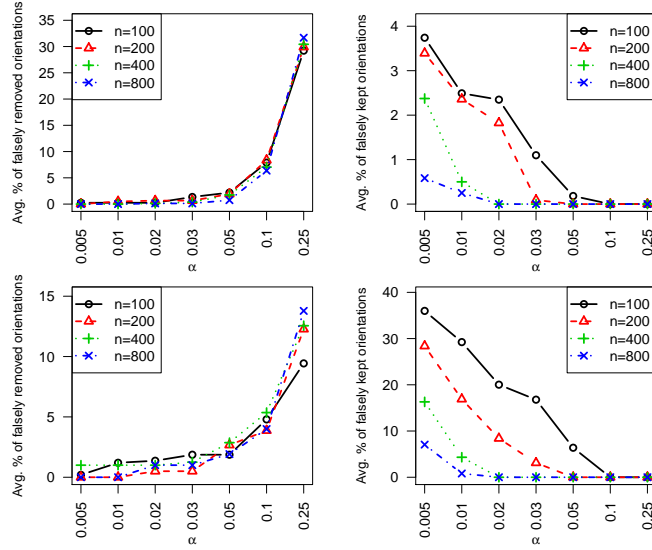


FIG 9. Performance of `computeGDPX` for varying sample sizes and values of α (x -axis) in sparse DAGs with $p_{\text{lin}} = 0.2$ (top) and $p_{\text{lin}} = 0.8$ (bottom). Parameters: $p = 10$, $n_{\text{rep}} = 100$ and $p_c = 2/9$ (expected number of edges: 10).

all settings. As demonstrated in Figure 11, the accuracy of `computeGDPX` with respect to varying values of α is barely affected by the number of variables p . In particular, `computeGDPX` exhibits a good performance even in high-dimensional settings with $p = 1000$ and sample sizes in the hundreds. The same conclusions hold for $p_c = 6/(p - 1)$ with an expected node degree of 6 (not shown).

4.5. Computation time

Lastly, we analyze the computation time of `computeGDPX` depending on the number of variables p and sparsity p_c . We examine two scenarios: (i) most of the functions in the PLSEM are nonlinear ($p_{\text{lin}} = 0.2$) and (ii) the worst-case scenario (w.r.t. computation time) where all the functions in the PLSEM are linear ($p_{\text{lin}} = 1$) and $\mathcal{D}(\mathbb{P})$ is equal to the Markov equivalence class ($G_{\mathcal{D}(\mathbb{P})}$ equals the CPDAG). For all combinations of $p \in \{10, 20, 50, 100, 250, 500, 1000, 2000, 5000\}$ and $p_c \in \{2/(p - 1), 8/(p - 1)\}$ and for both scenarios (i) and (ii), we measure the time consumption of `computeGDPX` for $n = 400$ and $\alpha = 0.05$. In the scenario where all the functions are linear, we additionally compare it to `dag2cpdag` in the R-package `pcalg`, which constructs the CPDAG based on iterative application of R1-R3 in Figure 6. The median CPU times are shown in Table 1. `computeGDPX` is able to estimate $G_{\mathcal{D}(\mathbb{P})}$ in less than a minute even if the number of variables is in the thousands. In general, the speed of our implementation heavily depends on the sparsity of the DAGs. This can be seen from the case with $p = 10$ and expected number of edges 40. In this setting the DAGs are

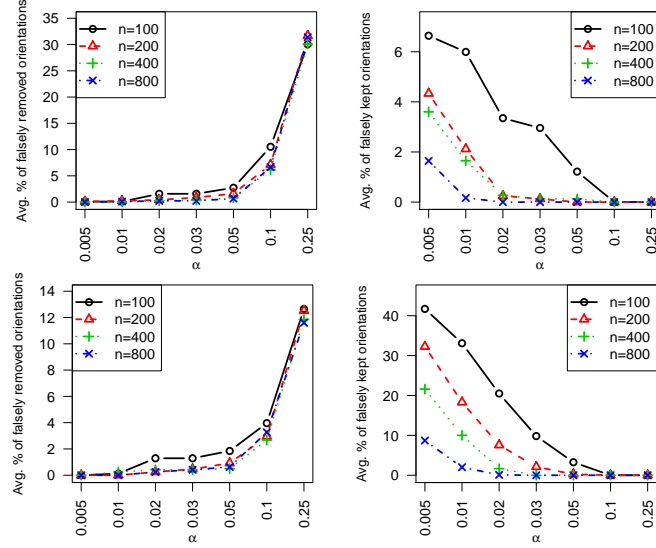


FIG 10. Performance of `computeGDPX` for varying sample sizes and values of α (x -axis) in dense DAGs for $p_{lin} = 0.2$ (top) and $p_{lin} = 0.8$ (bottom). Parameters: $p = 10$, $n_{rep} = 100$ and $p_c = 6/9$ (expected number of edges: 30).

almost fully connected. This in turn implies that not many of the edges are fixed due to v -structures and a lot of score-based tests have to be performed. On the other hand, if the underlying DAGs are sparse, we observe that `computeGDPX` even outperforms `dag2cpdag` with respect to computation time if the number of variables is large. Note that this only holds for sparse DAGs. In general, `dag2cpdag` is much faster than our implementation (not shown).

TABLE 1
Median CPU times [s] for `computeGDPX` and for `dag2cpdag` that iteratively applies $R1$ to $R3$ in Figure 6. $n_{rep} = 100$ repetitions for $p_{lin} = 0.2$ and $n_{rep} = 20$ repetitions for $p_{lin} = 1$.

$\mathbb{E}[\text{edges}]$	$p_{lin} = 0.2$		$p_{lin} = 1$			
	<code>computeGDPX</code>		<code>computeGDPX</code>		<code>dag2cpdag</code>	
	p	$4p$	p	$4p$	p	$4p$
$p = 10$	0.092	0.785	0.157	1.101	0.007	0.005
$p = 20$	0.150	0.105	0.174	0.162	0.006	0.006
$p = 50$	0.300	0.164	0.332	0.223	0.008	0.009
$p = 100$	0.604	0.281	0.665	0.325	0.014	0.016
$p = 250$	1.446	0.630	1.740	0.717	0.072	0.087
$p = 500$	2.705	1.253	3.486	1.523	0.395	0.599
$p = 1000$	5.616	2.513	6.603	2.974	3.464	4.231
$p = 2000$	11.504	5.380	13.493	6.331	25.463	31.591
$p = 5000$	29.226	16.276	35.094	18.462	400.324	591.574

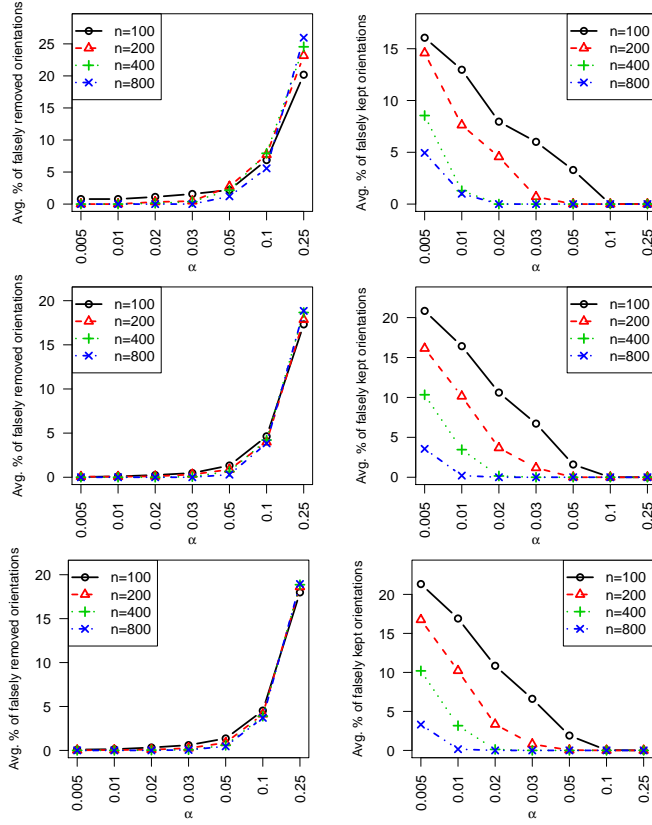


FIG 11. Performance of *computeGDPX* for varying sample sizes and values of α (x-axis) for $p = 10$ (top), $p = 100$ (middle) and $p = 1000$ (bottom). Parameters: $p_{in} = 0.5$, $n_{rep} = 100$ and $p_c = 2/9$ (expected number of edges: p).

5. Conclusion

We comprehensively characterized the identifiability of partially linear structural equation models with Gaussian noise (PLSEMs) from various perspectives. First, we proved that under faithfulness we obtain graphical and transformational characterizations of distribution equivalent DAGs similar to well-known characterizations of Markov equivalence classes of DAGs. More generally, we demonstrated that reinterpreting PLSEMs as PLSEM-functions leads to an interesting geometric characterization of all PLSEMs that generate the same distribution \mathbb{P} , as they can all be expressed as constant rotations of each other. Therefrom we derived a precise condition how PLSEM-functions (and hence also how single nonlinear additive components in PLSEMs) restrict the set of potential causal orderings of the variables and showed how it can be leveraged to conclude about the causal relations of specific pairs of variables under mild

additional assumptions. The theoretical results are complemented with an efficient algorithm that finds all equivalent DAGs to a given DAG or PLSEM. We proved its high-dimensional consistency and evaluated its performance on simulated data.

These characterizations of PLSEMs (and corresponding DAGs) that generate the same distribution \mathbb{P} are crucial for further algorithmic developments in structure learning, for example in the spirit of [4], or for Monte Carlo sampling in Bayesian settings, see a related discussion in [1, Section 1].

Appendix A: Proofs

This section contains detailed specifications and proofs of our main theorems. The order of the presentation matches the one in the main paper. Figure 12 gives an overview of the dependency structure of the different theorems.

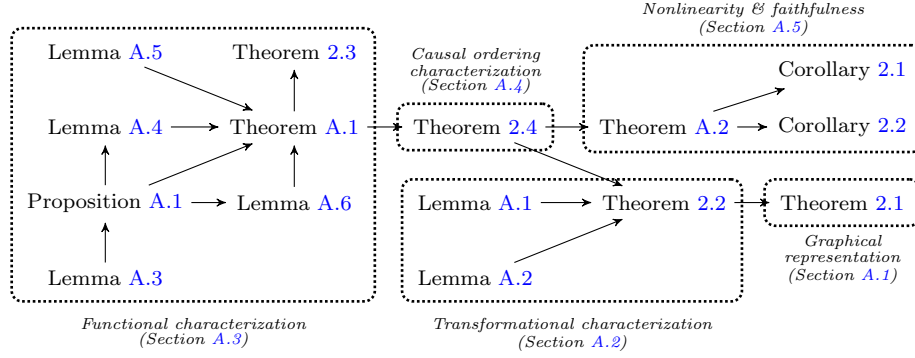


FIG 12. Proof structure for the characterization results in Section 2. The proofs for Section 3 are given in Appendix A.6 (not depicted).

A.1. Proof of the graphical characterization (Theorem 2.1)

Proof. By definition, $\mathcal{D}(\mathbb{P})$ is a subset of the set of all consistent DAG extensions of $G_{\mathcal{D}(\mathbb{P})}$. It remains to show, that the set of all consistent DAG extensions of $G_{\mathcal{D}(\mathbb{P})}$ is a subset of $\mathcal{D}(\mathbb{P})$. Suppose there is a consistent DAG extension \tilde{D} of $G_{\mathcal{D}(\mathbb{P})}$ such that $\tilde{D} \notin \mathcal{D}(\mathbb{P})$. Let $D \in \mathcal{D}(\mathbb{P})$. As both, D and \tilde{D} are consistent DAG extensions of $G_{\mathcal{D}(\mathbb{P})}$, they have the same skeleton and v -structures and are Markov equivalent. Hence, there exists a sequence of distinct covered edge reversals transforming D into \tilde{D} [6, Theorem 2]. Let us denote the sequence of traversed DAGs by $D = D_1, \dots, D_m = \tilde{D}$. If all covered edge reversals are linear, $\tilde{D} \in \mathcal{D}(\mathbb{P})$ by Theorem 2.2 (a), which contradicts the assumption. Therefore, there is at least one covered nonlinear edge reversal in this sequence. Without loss of generality, for $1 \leq r \leq m - 1$, let the edge reversal of $i \rightarrow j$ to $i \leftarrow j$ between D_r and D_{r+1} be the first covered nonlinear edge reversal in the above

sequence. First note that as the sequence of covered edge reversals is distinct, $i \rightarrow j$ in D and $i \leftarrow j$ in \tilde{D} . Moreover, as D_r is obtained from D by a sequence of covered linear edge reversals, $D_r \in \mathcal{D}(\mathbb{P})$ by Theorem 2.2 (a). Again, by Theorem 2.2 (a), as $D_r \in \mathcal{D}(\mathbb{P})$ and $i \rightarrow j$ is covered and nonlinear in D_r , $i \rightarrow j$ for all DAGs $D' \in \mathcal{D}(\mathbb{P})$. Therefore, by Definition 2.1, $i \rightarrow j$ in $G_{\mathcal{D}(\mathbb{P})}$ which contradicts the assumption that \tilde{D} is a consistent DAG extension of $G_{\mathcal{D}(\mathbb{P})}$. \square

A.2. Proof of transformational characterization (Theorem 2.2)

Proof. Part (a): By Lemma A.2 there exists a unique PLSEM with DAG D that generates \mathbb{P} . Let F denote the function that corresponds to this PLSEM as defined in Section 2.2.1. Without loss of generality let us assume that DF is lower triangular. Furthermore, as $i \rightarrow j$ is covered in D , no other child of i is an ancestor of j and we can assume that $j = i + 1$. The differential DF is of the form

$$\begin{pmatrix} \text{Var}(\varepsilon_1)^{-1/2} & 0 & \dots & \dots & \dots & 0 \\ \partial_1 F_2 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \text{Var}(\varepsilon_i)^{-1/2} & 0 & \ddots & \vdots \\ \vdots & \ddots & \partial_i F_{i+1} & \text{Var}(\varepsilon_{i+1})^{-1/2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \partial_1 F_p & \dots & \dots & \dots & \dots & \text{Var}(\varepsilon_p)^{-1/2} \end{pmatrix}.$$

Let us write $v = (DF)^{-1} \partial_i^2 F$, i.e. $\partial_i^2 F = DFv$. As DF is lower triangular with $(\text{Var}(\varepsilon_i)^{-1/2})_{i=1,\dots,p}$ on the diagonal we get $v_1, \dots, v_i = 0$ and $v_{i+1} = \text{Var}(\varepsilon_{i+1})^{1/2} \partial_i^2 F_{i+1}$. Hence,

$$e_{i+1}^t (DF)^{-1} \partial_i^2 F = \text{Var}(\varepsilon_{i+1})^{1/2} \partial_i^2 F_{i+1}.$$

Now recall that by definition of F ,

$$\partial_i^2 F_{i+1} = -\frac{1}{\text{Var}(\varepsilon_{i+1})^{1/2}} \partial_i^2 f_{i+1,i}(x_i).$$

By combining these two equations,

$$e_{i+1}^t (DF)^{-1} \partial_i^2 F = -\partial_i^2 f_{i+1,i}(x_i). \quad (\text{A.1})$$

By Lemma A.1, the edge can be reversed if and only if $(i, i+1) \notin \mathcal{V}$, which by definition of \mathcal{V} is the case if and only if

$$e_{i+1}^t (DF)^{-1} \partial_i^2 F \equiv 0.$$

By equation (A.1) this is the case if and only if $\partial_i^2 f_{i+1,i}(x_i) \equiv 0$. Hence the edge can be reversed if and only if the edge is linear. This concludes the proof of the

“if and only if” statement.

If the edge $i \rightarrow i + 1$ is nonlinear, we can argue analogously as above that $(i, i + 1) \in \mathcal{V}$. By Theorem 2.4, all causal orderings of PLSEMs that generate \mathbb{P} satisfy $\sigma(i) < \sigma(i + 1)$. As, by definition, \mathbb{P} is faithful to all DAGs in $\mathcal{D}(\mathbb{P})$, they all have the same skeleton. Hence, $i \rightarrow i + 1$ in all DAGs in $\mathcal{D}(\mathbb{P})$.

Part (b): As $D, D' \in \mathcal{D}(\mathbb{P})$, D' is Markov equivalent to D . Hence, there exists a sequence of distinct covered edge reversals transforming D into D' [6, Theorem 2]. Let us denote the sequence of traversed DAGs by $D = D_1, \dots, D_m = D'$. By part (a), we are done if we can show that each DAG D_r in this sequence lies in $\mathcal{D}(\mathbb{P})$. We prove this by induction. So let us assume $D_r \in \mathcal{D}(\mathbb{P})$ with $r < m$. Then D_{r+1} only differs from D_r by the reversal of a covered edge, w.l.o.g. $i \rightarrow j$ in D_r and $j \rightarrow i$ in D_{r+1} . By construction, all covered edge reversals are distinct, hence, $j \rightarrow i$ in D' . Define the set \mathcal{V} as in Theorem 2.4. As $D, D' \in \mathcal{D}(\mathbb{P})$, by Theorem 2.4, $(i, j) \notin \mathcal{V}$. Hence by Lemma A.1 we immediately get that $D_{r+1} \in \mathcal{D}(\mathbb{P})$. Moreover, by Theorem 2.2 (a), $i \rightarrow j$ is linear. This concludes the proof. \square

Lemma A.1. *Let $D \in \mathcal{D}(\mathbb{P})$. Let $i \rightarrow j$ be a covered edge in D . Let D' be a DAG that differs from D only by reversing $i \rightarrow j$. Let F be a PLSEM-function of \mathbb{P} and define \mathcal{V} as in equation (2.5). Then $D' \in \mathcal{D}(\mathbb{P})$ if and only if $(i, j) \notin \mathcal{V}$.*

Proof. “ \Rightarrow ”: Let $D' \in \mathcal{D}(\mathbb{P})$ and $(i, j) \in \mathcal{V}$. Consider a causal ordering σ of D' . As $j \rightarrow i$ in D' , $\sigma(j) < \sigma(i)$. By Theorem 2.4 this leads to a contradiction. Hence if $D' \in \mathcal{D}(\mathbb{P})$, then $(i, j) \notin \mathcal{V}$.

“ \Leftarrow ”: Let $(i, j) \notin \mathcal{V}$. Let σ be a causal ordering of D . As $i \rightarrow j$ is covered in D , no other child of i is an ancestor of j in D . Hence without loss of generality we can assume that $\sigma(j) = \sigma(i) + 1$. Define σ' as the permutation with i and j switched, i.e.

$$\sigma'(k) = \begin{cases} \sigma(k) & k \notin \{i, j\} \\ \sigma(j) & k = i \\ \sigma(i) & k = j. \end{cases}$$

Note that as $\sigma(j) = \sigma(i) + 1$, the causal orderings of other pairs of variables are unaffected, i.e.

$$\sigma(k) < \sigma(l) \iff \sigma'(k) < \sigma'(l) \text{ for all } k, l \text{ with } \{k, l\} \neq \{i, j\}. \quad (\text{A.2})$$

As σ is a causal ordering of a PLSEM that generates \mathbb{P} , by Theorem 2.4,

$$\sigma(k) < \sigma(l) \text{ for all } (k, l) \in \mathcal{V}. \quad (\text{A.3})$$

We want to show that the same holds for σ' . Let $(k, l) \in \mathcal{V}$. As $(i, j) \notin \mathcal{V}$, $(k, l) \neq (i, j)$. Hence, by equations (A.2) and (A.3), $\sigma'(k) < \sigma'(l)$. This proves that

$$\sigma'(k) < \sigma'(l) \text{ for all } (k, l) \in \mathcal{V}.$$

By Theorem 2.4, σ' is a causal ordering of a PLSEM that generates \mathbb{P} . Consider the DAG \tilde{D} of this PLSEM. Then \mathbb{P} is Markov with respect to \tilde{D} and by Proposition 17 of [17], \mathbb{P} satisfies causal minimality with respect to \tilde{D} . By [6, Lemma 1], \mathbb{P} is Markov and faithful with respect to D' and we know that σ' is a causal ordering of both \tilde{D} and D' . Now we want to show that this implies $\tilde{D} = D'$. Without loss of generality assume $\sigma' = \text{Id}$. First, we want to show that $\text{pa}_{\tilde{D}}(l) \supseteq \text{pa}_{D'}(l)$ for all l . Fix l . Consider the parental set $\text{pa}_{\tilde{D}}(l)$ of l in \tilde{D} and let k be a parent of l in D' but not in \tilde{D} . As $\sigma' = \text{Id}$ is a causal ordering of D' , $k < l$, and as $\sigma' = \text{Id}$ is a causal ordering of \tilde{D} as well, k is not a descendant of l in \tilde{D} . As \mathbb{P} is Markov with respect to \tilde{D} ,

$$X_l \perp\!\!\!\perp X_k | X_{\text{pa}_{\tilde{D}}(l)}.$$

Hence, as \mathbb{P} is faithful to D' , l and k are d-separated by $\text{pa}_{\tilde{D}}(l)$ in D' . But k is a parent of l in D' , contradiction. Hence $\text{pa}_{\tilde{D}}(l) \supseteq \text{pa}_{D'}(l)$ for all l . \mathbb{P} satisfies causal minimality with respect to \tilde{D} , hence $\text{pa}_{\tilde{D}}(l) = \text{pa}_{D'}(l)$ for all l . This proves $\tilde{D} = D'$. Therefore, there exists a PLSEM with DAG D' that generates \mathbb{P} and \mathbb{P} is faithful with respect to D' . By definition, $D' \in \mathcal{D}(\mathbb{P})$. \square

Lemma A.2. *Let \mathbb{P} be generated by a PLSEM. Let $D \in \mathcal{D}(\mathbb{P})$. Then there exists a unique PLSEM (unique set of intercepts, edge functions and Gaussian error variances) with DAG D that generates \mathbb{P} .*

Proof. By definition of the distribution equivalence class $\mathcal{D}(\mathbb{P})$ there exists such a PLSEM with DAG D that generates \mathbb{P} . Now we will show that this PLSEM is unique. Consider another PLSEM with DAG D that generates \mathbb{P} . For a given node j we have

$$\mu_j + \sum_{i \in \text{pa}_D(j)} f_{j,i}(X_i) = \mathbb{E}[X_j | X_{\text{pa}_D(j)}] = \tilde{\mu}_j + \sum_{i \in \text{pa}_D(j)} \tilde{f}_{j,i}(X_i).$$

By definition of PLSEMs, the expectations of the $f_{j,i}(X_i)$ and $\tilde{f}_{j,i}(X_i)$ are zero, hence we have $\mu_j = \tilde{\mu}_j$. As $\sigma_k > 0$ for all $k \in \{1, \dots, p\}$, the density of X is positive on \mathbb{R}^p . Recall that by definition, $f_{j,i}$ and $\tilde{f}_{j,i}$ are continuous. Hence, for all $x \in \mathbb{R}^p$,

$$\begin{aligned} \sum_{i \in \text{pa}_D(j)} f_{j,i}(x_i) &= \lim_{\delta \rightarrow 0} E \left[\sum_{i \in \text{pa}_D(j)} f_{j,i}(X_i) | X \in B_\delta(x) \right] \\ &= \lim_{\delta \rightarrow 0} E \left[\sum_{i \in \text{pa}_D(j)} \tilde{f}_{j,i}(X_i) | X \in B_\delta(x) \right] = \sum_{i \in \text{pa}_D(j)} \tilde{f}_{j,i}(x_i), \end{aligned}$$

where $B_\delta(x)$ denotes the closed ball around x with radius δ . Take an arbitrary $i \in \text{pa}_D(j)$. By taking the derivative with respect to x_i on both sides of the equation we obtain

$$f'_{j,i}(x_i) = \tilde{f}'_{j,i}(x_i).$$

Hence there exists a constant c such that

$$f_{j,i}(x_i) = c + \tilde{f}_{j,i}(x_i).$$

By definition of PLSEMs, we have $\mathbb{E}[f_{j,i}(X_i)] = 0$ and $\mathbb{E}[\tilde{f}_{j,i}(X_i)] = 0$. Hence, $c = 0$ and $f_{j,i} = \tilde{f}_{j,i}$ for all $i \in \text{pa}_D(j)$. We just showed that $\mu_j = \tilde{\mu}_j$ and $f_{j,i} = \tilde{f}_{j,i}$. It remains to show that $\sigma_j = \tilde{\sigma}_j$:

$$\sigma_j^2 = \text{Var}\left(X_j - \mu_j - \sum_{i \in \text{pa}_D(j)} f_{j,i}(X_i)\right) = \text{Var}\left(X_j - \tilde{\mu}_j - \sum_{i \in \text{pa}_D(j)} \tilde{f}_{j,i}(X_i)\right) = \tilde{\sigma}_j^2.$$

Hence, the intercepts, edge functions and Gaussian error variances of both PLSEMs are equal, which concludes the proof. \square

A.3. Proof of functional characterization (Theorem 2.3)

In the following, let \mathbb{P} be generated by a PLSEM.

Definition A.1 (PLSEM-functions). *We call $F : \mathbb{R}^p \rightarrow \mathbb{R}^p$ a PLSEM-function of \mathbb{P} if there exists a PLSEM that generates \mathbb{P} such that F can be written as in equation (2.1).*

Remark A.1. *For a PLSEM-function F of \mathbb{P} we can retrieve the unique corresponding PLSEM (i.e. the unique DAG, unique set of intercepts, edge functions and Gaussian error variances) through equations (2.2), (2.3) and (2.4).*

Proposition A.1. *A function $F : \mathbb{R}^p \rightarrow \mathbb{R}^p$ is a PLSEM-function of \mathbb{P} if and only if*

1. F is twice continuously differentiable,
2. $\partial_k \partial_l F \equiv 0$ for all $k \neq l$,
3. there exists a permutation σ such that $(DF_{i\sigma^{-1}(j)})_{ij}$ is lower triangular with constant positive entries on the diagonal.
4. If $X \sim \mathbb{P}$, then $F(X) \sim \mathcal{N}(0, Id_p)$,

We call a permutation σ that satisfies (3) a causal ordering of the PLSEM-function F . Define the directed graph D , the functions $f_{j,i}$, $\sigma_j^2 = \text{Var}(\varepsilon_j)$ and μ_j through equations (2.2) – (2.4). The first condition reflects that the functions $f_{j,i}$ are twice continuously differentiable. The second condition reflects that the functions $f_{j,i}$ depend on x_i only. The third condition ensures that the directed graph D is acyclic and that the variances of all ε_j are strictly positive. The last condition ensures that the distribution generated by this PLSEM is \mathbb{P} .

Proof. “ \Rightarrow ” By definition of a PLSEM and equation (2.1).

“ \Leftarrow ”: Without loss of generality let us assume that the indices are ordered such that $\sigma = \text{Id}$, hence by (3), DF is lower triangular with constant positive entries on the diagonal. Let $Z \sim \mathcal{N}(0, Id_p)$ and define $X := F^{-1}(Z)$. Using (4), we obtain $X \sim \mathbb{P}$. Use (1) and (2) and Lemma A.3 for each component of F_j ,

i.e. decompose $F_j(x) = \tilde{\mu}_j + \sum_i \tilde{f}_{j,i}(x_i)$ with twice continuously differentiable functions $\tilde{f}_{j,i}$. Here we choose $\tilde{\mu}_j$ and the $\tilde{f}_{j,i}$ (i.e. the constants) such that $\mathbb{E}[\tilde{f}_{j,i}(X_i)] \equiv 0$ for all $j \neq i$ and $\tilde{f}_{j,j}$ such that $\tilde{f}_{j,j}(0) = 0$. We define the parental sets $\text{pa}(j) := \{i \neq j : \tilde{f}_{j,i} \neq 0\}$. As DF is lower triangular, $\text{pa}(j) \subseteq \{1, \dots, j-1\}$, hence the directed graph D defined by these parental sets is acyclic. As DF has constant positive entries on the diagonal, $\partial_j F_j$ is constant, and we can define the error variances $\sigma_j^2 := 1/(\partial_j F_j)^2 > 0$. Furthermore, define functions $f_{j,i}(x_i) := -\sigma_j \tilde{f}_{j,i}(x_i)$ that only depend on x_i and the constants $\mu_j := -\sigma_j \tilde{\mu}_j$. To sum it up, we have the following relations:

$$F_j(x) = \frac{1}{\sigma_j} \left(x_j - \mu_j - \sum_{i \in \text{pa}_D(j)} f_{j,i}(x_i) \right),$$

with DAG D , $f_{j,i} \neq 0$, $\mathbb{E}[f_{j,i}(X_i)] = 0$ for all $i \in \text{pa}_D(j)$. Using that $F(X) = Z \sim \mathcal{N}(0, \text{Id}_p)$,

$$X_j = \mu_j + \sum_{i \in \text{pa}_D(j)} f_{j,i}(X_i) + \sigma_j Z_j$$

By defining the Gaussian errors $\varepsilon_j := \sigma_j Z_j$, it is immediate to see that $\sigma_j, f_{j,i}, D$ define a PLSEM that generates \mathbb{P} . \square

Theorem A.1 (Functional characterization). *Consider a PLSEM-function F of \mathbb{P} . Let σ be a permutation. Define Π_{i+1}^σ as the linear projection on the space $\langle \partial_{\sigma^{-1}(i+1)} F, \dots, \partial_{\sigma^{-1}(p)} F \rangle$ and $\Pi_{p+1}^\sigma := 0 \in \mathbb{R}^{p \times p}$. Let $G : \mathbb{R}^p \rightarrow \mathbb{R}^p$. Then G is a PLSEM-function of \mathbb{P} with causal ordering σ if and only if*

$$(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)}^2 F \equiv 0, \quad i = 1, \dots, p,$$

and

$$G_i = \left(\frac{(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F}{\|(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F\|_2} \right)^t F. \quad (\text{A.4})$$

In that case, the matrices Π_{i+1}^σ and the vectors $(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$ are constant.

Remark A.2. *This theorem tells us that every potential causal ordering satisfies $(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)}^2 F \equiv 0$, $i = 1, \dots, p$ and contains a concrete formula to compute the unique PLSEM-function for this given causal ordering. Furthermore, every causal ordering that satisfies that condition gives rise to a corresponding PLSEM-function by equation (A.4). As F is a PLSEM-function, DF is invertible. This implies $\|(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F\|_2 > 0$ and hence equation (A.4) is well-defined. Given the PLSEM-function, we can retrieve the unique corresponding PLSEM (i.e. the unique DAG, unique set of intercepts, edge functions and Gaussian error variances) through equations (2.2) – (2.4).*

Remark A.3. *If G is a PLSEM-function, from this theorem it follows that the vectors*

$$\left(\frac{(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F}{\|(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F\|_2} \right)^t \quad i = 1, \dots, p,$$

are constant in x , have norm 1 and are orthogonal for $i = 1, \dots, p$. Hence the row-wise concatenation of these vectors for $i = 1, \dots, p$ forms an orthogonal matrix O and by equation (A.4), $G = OF$.

Proof. “ \Rightarrow ”. Let G be a PLSEM-function of \mathbb{P} with causal ordering σ . Without loss of generality let $\sigma = \text{Id}$, i.e. without loss of generality we assume that DG is lower triangular. We write Π_{i+1} instead of Π_{i+1}^σ for brevity. Define $J := G(F^{-1})$. By Proposition A.1 (3), $\det DG$ and $\det DF$ are constant. Hence, $\det DJ$ is constant, too. Furthermore, by Proposition A.1 (4), $J(\varepsilon) \sim \mathcal{N}(0, \text{Id}_p)$ for $\varepsilon \sim \mathcal{N}(0, \text{Id}_p)$. By Lemma A.5 we obtain

$$\|G(x)\|_2^2 = \|F(x)\|_2^2 \text{ for all } x \in \mathbb{R}^p.$$

By differentiating on both sides,

$$G^t DG = F^t DF.$$

We assumed without loss of generality that $\sigma = \text{Id}$, hence by Proposition A.1 the differential DG is lower triangular and the diagonal entries $c_i := \partial_i G_i$ are positive. Hence we can recursively solve for $i = 1, \dots, p$ and obtain

$$G_i = \frac{1}{c_i} \left(F^t \partial_i F - \sum_{j>i} G_j \partial_i G_j \right) \quad (\text{A.5})$$

Using induction, we will show that

$$c_i G_i = F^t (\text{Id} - \Pi_{i+1}) \partial_i F, \quad (\text{A.6})$$

that $c_i = \|(\text{Id} - \Pi_{i+1}) \partial_i F\|_2$, that the matrix Π_{i+1} is constant and that the vectors $(\text{Id} - \Pi_{i+1}) \partial_i^2 F \equiv 0$ for $i = 1, \dots, p$. By using equation (A.5) we obtain equation (A.6) for $i = p$ and by Lemma A.4 we obtain $(\text{Id} - \Pi_{p+1}) \partial_p^2 F = \partial_p^2 F \equiv 0$. Hence,

$$c_p^2 = c_p \partial_p G_p = (\partial_p F)^t \partial_p F = \|(\text{Id} - \Pi_{p+1}) \partial_p F\|_2^2.$$

Furthermore, $(\text{Id} - \Pi_{p+1}) \partial_p F$ is a constant vector and hence by definition the matrix Π_p is constant. Now let us assume $c_j G_j = F^t (\text{Id} - \Pi_{j+1}) \partial_j F$, $c_j = \|(\text{Id} - \Pi_{j+1}) \partial_j F\|_2$, that the matrix Π_j is constant and that the vectors $(\text{Id} - \Pi_{j+1}) \partial_j^2 F \equiv 0$ for all $p \geq j > i \geq 1$. We want to prove these statements for $j = i$. By using equation (A.5) and the induction assumption we can rewrite $c_i G_i$,

$$\begin{aligned} c_i G_i &= F^t \partial_i F - \sum_{j>i} G_j \partial_i G_j \\ &= F^t \partial_i F - \sum_{j>i} \frac{F^t (\text{Id} - \Pi_{j+1}) \partial_j F}{c_j} \frac{\partial_i F^t (\text{Id} - \Pi_{j+1}) \partial_j F}{c_j} \\ &= F^t \left(\text{Id} - \sum_{j>i} \frac{(\text{Id} - \Pi_{j+1}) \partial_j F}{\|(\text{Id} - \Pi_{j+1}) \partial_j F\|_2} \frac{((\text{Id} - \Pi_{j+1}) \partial_j F)^t}{\|(\text{Id} - \Pi_{j+1}) \partial_j F\|_2} \right) \partial_i F \\ &= F^t (\text{Id} - \Pi_{i+1}) \partial_i F. \end{aligned}$$

By Lemma A.4 we get $(\text{Id} - \Pi_{i+1}) \partial_i^2 F \equiv 0$ and hence

$$\begin{aligned} c_i^2 &= c_i \partial_i G_i \\ &= \partial_i (F^t (\text{Id} - \Pi_{i+1}) \partial_i F) \\ &= \partial_i F^t (\text{Id} - \Pi_{i+1}) \partial_i F + 0 \\ &= \|(\text{Id} - \Pi_{i+1}) \partial_i F\|_2^2. \end{aligned}$$

It remains to show that Π_i is constant. We proved that $(\text{Id} - \Pi_{i+1}) \partial_i^2 F \equiv 0$. Π_{i+1} is constant by induction assumption. Thus, $\partial_i ((\text{Id} - \Pi_{i+1}) \partial_i F) \equiv 0$. By Proposition A.1 (2), $\partial_i F$ depends only on x_i . Hence the vector $(\text{Id} - \Pi_{j+1}) \partial_j F$ is constant for $j = i$. By induction assumption we also know that this is true for all $j > i$. By definition, we know that

$$\Pi_i = \sum_{j \geq i} \frac{(\text{Id} - \Pi_{j+1}) \partial_j F}{\|(\text{Id} - \Pi_{j+1}) \partial_j F\|_2} \frac{((\text{Id} - \Pi_{j+1}) \partial_j F)^t}{\|(\text{Id} - \Pi_{j+1}) \partial_j F\|_2}.$$

As shown, the quantities on the right-hand side are constant. This concludes the proof by induction.

“ \Leftarrow ” We will show 1) – 4) of Proposition A.1 to prove that G is a PLSEM-function of \mathbb{P} . By Lemma A.6, the vectors $(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$ are constant. As F is twice continuously differentiable, G is twice differentiable as well. This proves 1). By part 2) of Proposition A.1, $\partial_k \partial_l F = 0$ for all $k \neq l$. Recall that the vector $(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$ is constant. Let $k \neq l$. Hence $\partial_k \partial_l G_i = (\partial_k \partial_l F)^t (\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F / \|(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F\|_2 = 0$. This proves that for all $k \neq l$, $\partial_k \partial_l G = 0$, i.e. part 2) of Proposition A.1. Now we want to show that $(DG_{i\sigma^{-1}(j)})_{ij}$ is lower triangular. By construction, $DG_{i\sigma^{-1}(j)} = \partial_{\sigma^{-1}(j)} G_i = \partial_{\sigma^{-1}(j)} F^t (\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F = 0$ for all $j > i$ as by definition $\partial_{\sigma^{-1}(j)} F^t (\text{Id} - \Pi_{i+1}^\sigma) = 0$. Now we want to show that $(DG_{i\sigma^{-1}(j)})_{ij}$ has positive constant entries on the diagonal. Recall that by assumption $(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)}^2 F \equiv 0$ for $i = 1, \dots, p$. Recall that the vector $(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$ is constant. The vector is nonzero as DF is invertible. Hence,

$$DG_{i\sigma^{-1}(i)} = \frac{\partial_{\sigma^{-1}(i)} F^t (\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F}{\|(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F\|_2} = \frac{\|(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F\|_2^2}{\|(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F\|_2}.$$

Thus $DG_{i\sigma^{-1}(i)}$ is constant. This proves 3). Let $X \sim \mathbb{P}$. Now it remains to show that $G(X) \sim \mathcal{N}(0, \text{Id})$. To this end, note that by definition of Π_{j+1}^σ , the vectors

$$(\text{Id} - \Pi_{j+1}^\sigma) \partial_{\sigma^{-1}(j)} F, j = 1, \dots, p,$$

are orthogonal. As shown above, these vectors are constant and nonzero, therefore $(\text{Id} - \Pi_{j+1}^\sigma) \partial_{\sigma^{-1}(j)} F, j = 1, \dots, p$ is an orthogonal basis of \mathbb{R}^p . Therefore, $\|F(x)\|_2^2 = \|G(x)\|_2^2$ for all $x \in \mathbb{R}^p$. As $\det DG$ is constant, we have by the change of variables formula that $|\det DG| = |\det DF|$ (probability densities integrate to one). Hence, again by the change of variables formula, $G(X) \sim \mathcal{N}(0, \text{Id})$, which is 4). This concludes the proof of the “if and only if” statement.

Lemma A.6 proves that in that case, the matrices Π_{i+1}^σ and the vectors $(\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$ are constant. This concludes the proof. \square

Lemma A.3. *Let $F : \mathbb{R}^p \mapsto \mathbb{R}$ be twice continuously differentiable. If $\partial_k \partial_l F \equiv 0$ for all $l \neq k$, then F can be written in the form*

$$F(x) = c + g_1(x_1) + \dots + g_p(x_p). \quad (\text{A.7})$$

In this case, the functions $g_i(x_i)$ are unique up to constants and twice continuously differentiable.

Proof. Fix an arbitrary $y \in \mathbb{R}^p$. We use Taylor:

$$\begin{aligned} F(x) - F(y) &= \int_{y_1}^{x_1} \partial_1 F(z, x_2, \dots, x_p) dz + \dots + \int_{y_p}^{x_p} \partial_p F(y_1, y_2, \dots, y_{p-1}, z) dz \\ &= \int_{y_1}^{x_1} \partial_1 F(z, 0, \dots, 0) dz + \dots + \int_{y_p}^{x_p} \partial_p F(0, 0, \dots, 0, z) dz \end{aligned}$$

In the second line we used that $\partial_k \partial_l F \equiv 0$ for all $l \neq k$. Now we can define

$$g_i(x_i) = \int_{y_i}^{x_i} \partial_i F(0, \dots, 0, z, 0, \dots, 0) dz,$$

which proves equation (A.7) with constant $c = F(y)$. Furthermore, as

$$\partial_i F = \partial_i g_i(x_i),$$

the g_i are unique up to constants. This completes the proof. \square

Lemma A.4. *Let $F, G : \mathbb{R}^p \rightarrow \mathbb{R}^p$ be PLSEM-functions of \mathbb{P} . Let Π be a constant projection matrix. If $c_i G_i = F^t (Id - \Pi) \partial_i F$ for a constant c_i , then*

$$(Id - \Pi) \partial_i^2 F \equiv 0.$$

Proof. Recall Proposition A.1. We will use properties 1), 2) and 3) of F and G in the proof. As G is a PLSEM-function, by Proposition A.1

$$\partial_j F^t (Id - \Pi) \partial_i^2 F = c_i \partial_i \partial_j G_i = 0 \text{ for all } j \neq i.$$

As Π is a projection matrix, we have $(Id - \Pi)^t (Id - \Pi) = (Id - \Pi)(Id - \Pi) = (Id - \Pi)$, which implies

$$((Id - \Pi) \partial_j F)^t (Id - \Pi) \partial_i^2 F = 0 \text{ for all } j \neq i. \quad (\text{A.8})$$

As F is a PLSEM-function, by Proposition A.1, there exists a permutation σ such that $(DF_{k\sigma^{-1}(l)})_{kl}$ is lower triangular with constant positive entries on the diagonal. Without loss of generality let us assume that $\sigma = Id$, i.e., that the variables x_i are ordered such that DF is lower triangular with constant positive entries on the diagonal. Hence $\langle \partial_p F, \dots, \partial_{i+1} F \rangle = \langle e_p, \dots, e_{i+1} \rangle$, and $\partial_i^2 F \in \langle e_p, \dots, e_{i+1} \rangle$. Furthermore, $\partial_i^2 F \in \langle \partial_p F, \dots, \partial_{i+1} F \rangle$ which implies $(Id - \Pi) \partial_i^2 F \in \langle (Id - \Pi) \partial_p F, \dots, (Id - \Pi) \partial_{i+1} F \rangle$. By equation (A.8), $(Id - \Pi) \partial_i^2 F \equiv 0$. \square

Lemma A.5. *Let $\varepsilon \sim \mathcal{N}(0, Id_p)$ and $J : \mathbb{R}^p \rightarrow \mathbb{R}^p$ be a \mathcal{C}^1 -diffeomorphism such that $\det DJ$ is constant and $J(\varepsilon) \sim \mathcal{N}(0, Id_p)$. Then, $|\det DJ| = 1$ and*

$$\|J(e)\|_2 = \|e\|_2 \text{ for all } e \in \mathbb{R}^p.$$

Proof. By assumption, for every Borel set $A \subset \mathbb{R}^p$, $\mathbb{P}[\varepsilon \in A] = \mathbb{P}[J^{-1}(\varepsilon) \in A]$. Hence, by the change of variables formula,

$$\begin{aligned} \int_A \frac{1}{(\sqrt{2\pi})^p} \exp\left(-\frac{\|\varepsilon\|_2^2}{2}\right) d\varepsilon &= \int_{J(A)} \frac{1}{(\sqrt{2\pi})^p} \exp\left(-\frac{\|\varepsilon\|_2^2}{2}\right) d\varepsilon \\ &= \int_A |\det DJ| \frac{1}{(\sqrt{2\pi})^p} \exp\left(-\frac{\|J(\varepsilon)\|_2^2}{2}\right) d\varepsilon. \end{aligned}$$

By continuity of J , for all $\varepsilon \in \mathbb{R}^p$, $\|\varepsilon\|_2^2 = \|J(\varepsilon)\|_2^2 - 2\log(|\det DJ|)$. As J is a diffeomorphism there exists an ε^0 such that $J(\varepsilon^0) = 0$. This immediately implies $\log(|\det DJ|) \leq 0$. Analogously, for $\varepsilon = 0$ we obtain $\log(|\det DJ|) \geq 0$. Hence, $\log(|\det DJ|) = 0$ and for all $\varepsilon \in \mathbb{R}^p$, $\|\varepsilon\|_2^2 = \|J(\varepsilon)\|_2^2$. This concludes the proof. \square

Lemma A.6. *Let F be a PLSEM-function and σ a permutation on $\{1, \dots, p\}$. Let*

$$(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)}^2 F \equiv 0, \text{ for } i = 1, \dots, p, \quad (\text{A.9})$$

where Π_{i+1}^σ denotes the linear projection on the space $\langle \partial_{\sigma^{-1}(i+1)} F, \dots, \partial_{\sigma^{-1}(p)} F \rangle$ and $\Pi_{p+1}^\sigma = 0 \in \mathbb{R}^{p \times p}$. Then the matrices Π_{i+1}^σ and vectors $(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$ are constant for $i = 1, \dots, p$.

Proof. Let us first show that the projection matrices Π_{i+1}^σ are constant. For $i = p$ the claim is trivial as $\Pi_{p+1}^\sigma \equiv 0$ and hence by equation (A.9), $\partial_{\sigma^{-1}(p)}^2 F \equiv 0$. For arbitrary i , equation (A.9) implies that $\partial_{\sigma^{-1}(i)}^2 F \in \langle \partial_{\sigma^{-1}(i+1)} F, \dots, \partial_{\sigma^{-1}(p)} F \rangle$. Furthermore, as F is a PLSEM-function, by Proposition A.1, $\partial_{\sigma^{-1}(i)} F$ only depends on $x_{\sigma^{-1}(i)}$. Using these two facts it follows inductively for $i = p-1, \dots, 1$ that the linear spaces $\langle \partial_{\sigma^{-1}(i+1)} F, \dots, \partial_{\sigma^{-1}(p)} F \rangle$, $i = p-1, \dots, 1$ are constant in x . Hence the linear projections on these spaces are constant matrices. This proves that the matrices Π_{i+1}^σ , $i = 1, \dots, p$ are constant. Now we want to show that the vectors $(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$, $i = 1, \dots, p$ are constant. Recall that $\partial_{\sigma^{-1}(i)} F$ only depends on $x_{\sigma^{-1}(i)}$. Hence $(Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F$ can only depend on $x_{\sigma^{-1}(i)}$. Hence it suffices to show that $\partial_{\sigma^{-1}(i)} (Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F = 0$. By equation (A.9) and as the matrix Π_{i+1}^σ is constant, $\partial_{\sigma^{-1}(i)} (Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)} F = (Id - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)}^2 F = 0$. This concludes the proof. \square

A.4. Proof of characterization via causal orderings (Theorem 2.4)

Remark A.4. *Slight abuse of notation. A priori, \mathcal{V} might depend on the concrete choice of F . However by Theorem 2.4, the set of permutations $\{\sigma : \sigma(i) < \sigma(k) \text{ for all } (i, k) \in \mathcal{V}\}$ does only depend on \mathbb{P} .*

Proof. Let Π_{i+1}^σ be the linear projection on the space $\langle \partial_{\sigma^{-1}(i+1)}F, \dots, \partial_{\sigma^{-1}(p)}F \rangle$ and $\Pi_{p+1}^\sigma := 0 \in \mathbb{R}^{p \times p}$. By some algebra,

$$\begin{aligned} & (\text{Id} - \Pi_{i+1}^\sigma) \partial_{\sigma^{-1}(i)}^2 F \equiv 0 \text{ for all } i \\ \iff & \partial_{\sigma^{-1}(i)}^2 F(x) \in \langle \partial_{\sigma^{-1}(i+1)}F(x), \dots, \partial_{\sigma^{-1}(p)}F(x) \rangle \text{ for all } i, \text{ for all } x \in \mathbb{R}^p \\ \iff & e_{\sigma^{-1}(j)}^t (DF)^{-1} \partial_{\sigma^{-1}(i)}^2 F \equiv 0 \text{ for all } j \leq i \\ \iff & j > i \text{ for all } e_{\sigma^{-1}(j)}^t (DF)^{-1} \partial_{\sigma^{-1}(i)}^2 F \neq 0 \\ \iff & \sigma(j) > \sigma(i) \text{ for all } e_j^t (DF)^{-1} \partial_i^2 F \neq 0. \end{aligned}$$

Here, $e_j, j = 1, \dots, p$ denotes the standard basis of \mathbb{R}^p . By invoking Theorem A.1 and Remark A.2 the assertion follows. \square

A.5. Interplay of nonlinearity and faithfulness (Corollaries 2.1 & 2.2)

Let $C_i := \{j \text{ child of } i \text{ in } D : \partial_i^2 f_{j,i} \neq 0\}$ be the set of nonlinear children of i . Define \mathcal{V} as in equation (2.5) and consider the condition

$$\text{The functions } f_{j,i}, j \in C_i \text{ are linearly independent.} \quad (\text{A.10})$$

Theorem A.2 (Nonlinear descendants are identifiable under minor assumptions). *Consider a PLSEM with DAG D that generates \mathbb{P} and the corresponding PLSEM-function F . Define \mathcal{V} and C_i as above. Fix $i \in \{1, \dots, p\}$. Then:*

- (a) *Let equation (A.10) hold and let $j \in C_i$. Then $(i, j) \in \mathcal{V}$.*
- (b) *Let $(i, j) \in \mathcal{V}$. Then j is a descendant of i in every DAG D' of a PLSEM that generates \mathbb{P} .*
- (c) *Let \mathbb{P} be faithful to D and let equation (A.10) hold. Consider a descendant k of i , $k \neq i$. Then $(i, k) \in \mathcal{V}$ if and only if k is descendant of one of the nonlinear children in C_i .*
- (d) *Define $\tilde{\mathcal{V}}$ as the transitive closure of \mathcal{V} . Let $k \neq i$. Then $(i, k) \in \tilde{\mathcal{V}}$ if and only if k is a descendant of i in every DAG D' of a PLSEM that generates \mathbb{P} .*

Remark A.5. We follow the convention that i is a descendant of itself. If equation (A.10) holds for all i , then from (c) it follows that $\tilde{\mathcal{V}} = \mathcal{V}$. In particular, by (d), k is descendant of one of the nonlinear children in C_i if and only if k is a descendant of i in every DAG D' of a PLSEM that generates \mathbb{P} .

Proof. We will first show (a) and (c). Recall Proposition A.1. Without loss of generality let us assume that $\sigma = \text{Id}$, i.e. that DF is lower triangular with constant positive entries on the diagonal. Furthermore, $\partial_i^2 F_l = 0$ for all $l \leq i$. Using this we obtain $(DF)^{-1} \partial_i^2 F = (DF)_{\bullet, (i+1):p}^{-1} \partial_i^2 F_{(i+1):p}$, and

$$\begin{aligned} e_k^t (DF)^{-1} \partial_i^2 F & \equiv 0 & (\text{A.11}) \\ \iff e_k^t (DF)_{\bullet, (i+1):p}^{-1} \partial_i^2 F_{(i+1):p} & \equiv 0. \end{aligned}$$

Here the subindex \bullet denotes all rows $1 : p$. In the next step, we want to prove that

$$\langle \partial_i^2 F_{(i+1):p}(x_i) \rangle_{x_i \in \mathbb{R}} = \langle (e_j)_{(i+1):p} \rangle_{j \in C_i}. \quad (\text{A.12})$$

Note that as the components $1, \dots, i$ of $\partial_i^2 F$ and $e_j, j \in C_i$ are zero, this is equivalent to showing that

$$\langle \partial_i^2 F(x_i) \rangle_{x_i \in \mathbb{R}} = \langle e_j \rangle_{j \in C_i}.$$

As $\partial_i^2 F_l \equiv 0$ for all $l \notin C_i$, we have

$$\langle \partial_i^2 F(x_i) \rangle_{x_i \in \mathbb{R}} \subseteq \langle e_j \rangle_{j \in C_i}.$$

Let $\gamma \in \langle e_j \rangle_{j \in C_i}$, $\gamma \neq 0$.

$$(\partial_i^2 F(x_i))^t \gamma = \sum_{j \in C_i} \partial_i^2 F_j(x_i) \gamma_j$$

As the nonlinear children in C_i are linearly independent, there exists an $x_i \in \mathbb{R}$ such that $\sum_j \partial_i^2 F_j(x_i) \gamma_j \neq 0$. Hence there exists no nonzero vector γ in $\langle e_j \rangle_{j \in C_i}$ that is orthogonal to $\langle \partial_i^2 F(x_i) \rangle_{x_i \in \mathbb{R}}$ and hence

$$\langle \partial_i^2 F(x_i) \rangle_{x_i \in \mathbb{R}} = \langle e_j \rangle_{j \in C_i}.$$

As discussed above, this proves equation (A.12). By Proposition A.1, each column l of DF is a function of x_l (i.e. constant in $x_1, \dots, x_{l-1}, x_{l+1}, \dots, x_p$). Hence, $(DF)_{\bullet, (i+1):p}^{-1}$ is a function of x_{i+1}, \dots, x_p . In particular, $(DF)_{\bullet, (i+1):p}^{-1}$ is constant in x_i . Now we can continue:

$$\begin{aligned} e_k^t (DF)_{\bullet, (i+1):p}^{-1} \partial_i^2 F_{i+1:p} &\equiv 0 & (\text{A.13}) \\ \iff e_k^t (DF)_{\bullet, (i+1):p}^{-1} (x_{i+1}, \dots, x_p) \partial_i^2 F_{i+1:p}(x_i) &= 0 \text{ for all } x \in \mathbb{R}^p \\ \iff e_k^t (DF)_{\bullet, (i+1):p}^{-1} (x_{i+1}, \dots, x_p) (e_j)_{(i+1):p} &= 0 \text{ for all } j \in C_i, x \in \mathbb{R}^p \\ \iff e_k^t (DF)^{-1}(x) e_j &= 0 \text{ for all } j \in C_i, x \in \mathbb{R}^p \end{aligned}$$

As DF is lower triangular with positive entries on the diagonal, $(DF)^{-1}$ is lower triangular too, with nonzero entries on the diagonal. Hence, $e_k^t (DF)^{-1}(x) e_k \neq 0$. So if $k \in C_i$, by equation (A.13), $e_k^t (DF)_{\bullet, (i+1):p}^{-1} \partial_i^2 F_{i+1:p} \neq 0$. By equation (A.11), $e_k^t (DF)^{-1} \partial_i^2 F \neq 0$ and hence by definition of \mathcal{V} , $(i, k) \in \mathcal{V}$. This proves (a).

Let $Z \sim \mathcal{N}(0, \text{Id}_p)$. Let $X = F^{-1}(Z)$. By Proposition A.1, $X \sim \mathbb{P}$. Note that $X_k = e_k^t F^{-1}(Z)$. We denote the partial derivative with respect to z_j by ∂_j^z . Note that x_k is constant in z_j if and only if $\partial_j^z e_k^t F^{-1}(z) = e_k^t (DF)^{-1}(F^{-1}(z)) e_j \equiv 0$. Fix j . As there are bijective relationships between x and z and between $x_{1:(j-1)}$

and $z_{1:(j-1)}$,

$$\begin{aligned}
& e_k^t(DF)^{-1}(x)e_j = 0 \quad \text{for all } x \in \mathbb{R}^p \tag{A.14} \\
& \iff e_k^t(DF)^{-1}(F^{-1}(z))e_j = 0 \quad \text{for all } z \in \mathbb{R}^p \\
& \iff x_k = e_k^t F^{-1}(z) \text{ is constant in } z_j \\
& \iff x_k = e_k^t F^{-1}(z) \text{ is a function of } z_1, \dots, z_{j-1}, z_{j+1}, \dots, z_k \\
& \Rightarrow X_k \perp\!\!\!\perp Z_j | Z_1, \dots, Z_{j-1} \\
& \Rightarrow X_k \perp\!\!\!\perp Z_j | X_1, \dots, X_{j-1} \\
& \Rightarrow X_k \perp\!\!\!\perp X_j | X_1, \dots, X_{j-1} \\
& \Rightarrow k \text{ is not a descendant of } j \text{ in } D.
\end{aligned}$$

In the second to last line we used that $X_j = \sum_{j' \in \text{pa}_D(j)} f_{j,j'}(X_{j'}) + \sigma_j Z_j$. In the last line we used faithfulness. The other direction follows from the definition of a PLSEM with DAG D : For all $j \in C_i$ we have that

$$k \text{ is a non-descendant of } j \text{ in } D \Rightarrow x_k = e_k^t F^{-1}(z) \text{ is constant in } z_j. \tag{A.15}$$

By combining equation (A.14) and equation (A.15),

$$e_k^t(DF)^{-1}(x)e_j = 0 \iff k \text{ is a non-descendant of } j \text{ in } D.$$

Hence, by equation (A.11) and equation (A.13)

$$\begin{aligned}
& k \text{ is a non-descendant of } j \text{ in } D \text{ for all } j \in C_i \\
& \iff e_k^t(DF)^{-1}_{\bullet, (i+1):p}(e_j)_{(i+1):p} \equiv 0 \text{ for all } j \in C_i \\
& \iff e_k^t(DF)^{-1} \partial_i^2 F \equiv 0.
\end{aligned}$$

This concludes the proof of (c). Now let us turn to the proof of (d).

Fix a DAG D' . k is a descendant of i in D' if and only if for all causal orderings σ of D' we have $\sigma(i) < \sigma(k)$. Hence,

$$\begin{aligned}
& k \text{ is a descendant of } i \text{ in all DAGs } D' \text{ of a PLSEM that generates } \mathbb{P} \\
& \iff \text{for all causal orderings } \sigma \text{ of a DAG } D' \text{ of a PLSEM} \tag{A.16} \\
& \text{that generates } \mathbb{P}: \sigma(i) < \sigma(k).
\end{aligned}$$

By Theorem 2.4 a permutation σ is a causal ordering of a DAG D' of a PLSEM that generates \mathbb{P} if and only if $\sigma(l) < \sigma(m)$ for all $(l, m) \in \mathcal{V}$:

$$\begin{aligned}
& \text{for all causal orderings } \sigma \text{ of a DAG } D' \text{ of a PLSEM} \\
& \text{that generates } \mathbb{P}: \sigma(i) < \sigma(k) \\
& \iff \text{for all permutations } \sigma \text{ with } \sigma(l) < \sigma(m) \text{ for all } (l, m) \in \mathcal{V} \tag{A.17} \\
& \text{we have } \sigma(i) < \sigma(k) \\
& \iff (i, k) \in \tilde{\mathcal{V}}.
\end{aligned}$$

Combining equations (A.16) and (A.17) concludes the proof of (d). (b) follows from (d): $(i, j) \in \mathcal{V}$ implies that $(i, j) \in \tilde{\mathcal{V}}$. This concludes the proof of (b). \square

A.6. Proofs of consistency and correctness of estimation procedures

A.6.1. Proof of Theorem 3.1

Proof. We prove that for n sufficiently large and with high probability, for any DAG $D^0 \in \mathcal{D}(\mathbb{P})$ and $D \in \mathcal{C}(D^0)$ such that (without loss of generality) D^0 and D only differ by reversal of a covered edge between nodes i and j ,

$$\log(\hat{\sigma}_i^D) + \log(\hat{\sigma}_j^D) - \log(\hat{\sigma}_i^{D^0}) - \log(\hat{\sigma}_j^{D^0}) \geq 3\xi_0/4, \quad (\text{A.18})$$

where $\hat{\sigma}_j^D$ denotes the unpenalized maximum likelihood estimator of the standard deviation of the residuals at node j in DAG D . Similarly, for n sufficiently large and with high probability, for $D^0, \tilde{D}^0 \in \mathcal{D}(\mathbb{P})$ that only differ by a reversal of a covered linear edge between nodes i and j ,

$$\left| \log(\hat{\sigma}_i^{D^0}) + \log(\hat{\sigma}_j^{D^0}) - \log(\hat{\sigma}_i^{\tilde{D}^0}) - \log(\hat{\sigma}_j^{\tilde{D}^0}) \right| \leq \xi_0/4. \quad (\text{A.19})$$

The uniform bounds in (A.18) and (A.19) imply that for $\alpha \in (\xi_0/4, 3\xi_0/4)$, each score-based decision whether a covered edge $i \rightarrow j$ is linear or not in step 6 of Algorithm 2 is consistent. The consistency of the estimated distribution equivalence class then follows from the correctness of Algorithm 1, which is justified at the beginning of Section 3.1. Obviously, the constants in (A.18) and (A.19) can be changed allowing for any $\alpha \in (0, \xi_0)$.

Proof of (A.18). By Assumption 3.1 (i), all DAGs under consideration have uniformly bounded node degrees. It now follows exactly along the lines of Sections 2.1, 2.2, 2.3 and 5 in the supplement to [3] that for $D \in \mathcal{D}(\mathbb{P}) \cup \mathcal{C}(\mathcal{D}(\mathbb{P}))$,

$$(\sigma_k^D)^2 \leq (\hat{\sigma}_k^D)^2 + \Delta_{n,k}^D, \quad (\text{A.20})$$

and for $D^0 \in \mathcal{D}(\mathbb{P})$,

$$(\hat{\sigma}_k^{D^0})^2 \leq (\sigma_k^{D^0})^2 + \gamma_{n,k}^{D^0} + \Delta_{n,k}^{D^0}, \quad (\text{A.21})$$

with $\Delta_{n,k}^D, \gamma_{n,k}^{D^0}$ as defined in Assumptions 3.1 (iii) and (iv).

Without loss of generality, let $D^0 \in \mathcal{D}(\mathbb{P})$ and $D \in \mathcal{C}(D^0)$ such that D^0 and D only differ by reversal of a covered nonlinear edge between nodes i and j . Substituting (A.20) and (A.21) and then using (3.1) and (3.2),

$$\begin{aligned} \sum_{k \in \{i,j\}} \left(\log(\hat{\sigma}_k^D) - \log(\hat{\sigma}_k^{D^0}) \right) &\geq \sum_{k \in \{i,j\}} \left(\log(\sigma_k^D) - \log(\sigma_k^{D^0}) \right) + R_{n,D,D^0} \\ &\geq \xi_p + R_{n,D,D^0}, \end{aligned}$$

where

$$R_{n,D,D^0} = \frac{1}{2} \sum_{k \in \{i,j\}} \left(\log \left(1 + \frac{-\Delta_{n,k}^D}{(\sigma_k^D)^2} \right) - \log \left(1 + \frac{\gamma_{n,k}^{D^0} + \Delta_{n,k}^{D^0}}{(\sigma_k^{D^0})^2} \right) \right).$$

By Assumption 3.1 (ii), the error variances are bounded away from zero. Using Taylor expansion and Assumptions 3.1 (iii) and (iv), $R_{n,D,D^0} = o_P(1)$. As ξ_p is uniformly bounded from below by ξ_0 , we have that

$$\sum_{k \in \{i,j\}} \left(\log(\hat{\sigma}_k^D) - \log(\hat{\sigma}_k^{D^0}) \right) \geq \xi_0 + o_P(1).$$

Therefore, for n sufficiently large and with high probability,

$$\sum_{k \in \{i,j\}} \left(\log(\hat{\sigma}_k^D) - \log(\hat{\sigma}_k^{D^0}) \right) \geq 3\xi_0/4.$$

A completely analogous argument yields (A.19) for $D^0, \tilde{D}^0 \in \mathcal{D}(\mathbb{P})$. \square

A.6.2. Proof of Lemma 3.1

Proof. (a) For a DAG D with $i \rightarrow j$ in D , we denote by $D_{i \leftarrow j}$ the graph that differs from D only by the reversal of $i \rightarrow j$. Let $i \rightarrow j$ in \mathcal{K} . Recall that $G_{P,\mathcal{K}}$ is obtained by imposing all edge orientations in \mathcal{K} on the pattern P and closing orientations under R1-R4 in Figure 6. Hence, by construction, $i \rightarrow j$ in $G_{P,\mathcal{K}}$. Throughout the proof we use that for a background knowledge \mathcal{K}' , by [12, Theorems 2&4], the set of all consistent DAG extensions of $G_{P,\mathcal{K}'}$ equals the set of all Markov equivalent DAGs that have pattern P and edge orientations that comply with the background knowledge \mathcal{K}' . Then, it holds that

$$\begin{aligned} & \exists \text{ consistent DAG extension } D \text{ of } G_{P,\mathcal{K}} \text{ in which } i \rightarrow j \text{ is covered} \\ \iff & \exists \text{ consistent DAG extension } D \text{ of } G_{P,\mathcal{K}}: D_{i \leftarrow j} \text{ is Markov} \\ & \text{equivalent to } D \\ \iff & \exists \text{ consistent DAG extension } D \text{ of } G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}: D_{i \leftarrow j} \text{ is Markov} \\ & \text{equivalent to } D, \end{aligned}$$

where the first equivalence follows from [6, Lemma 1]. By assumption, $i \rightarrow j$ is not in P and not in the background knowledge. Hence, the soundness of the four orientation rules R1-R4 [12, Theorem 2] implies that $i - j$ in $G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}$ which is the case if and only if $G_{P,\mathcal{K}} \neq G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}$.

To show the other implication, by the completeness of the orientation rules in [12, Theorem 4],

$$\begin{aligned} & i - j \text{ in } G_{P,\mathcal{K} \setminus \{i \rightarrow j\}} \\ \implies & \exists \text{ consistent DAG extensions } D_1, D_2 \text{ of } G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}: i \rightarrow j \text{ in } D_1 \text{ and} \\ & i \leftarrow j \text{ in } D_2 \\ \implies & \exists \text{ consistent DAG extension } D \text{ of } G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}: D_{i \leftarrow j} \text{ is a consistent DAG} \\ & \text{extension of } G_{P,\mathcal{K} \setminus \{i \rightarrow j\}}, \end{aligned}$$

where the last implication follows from [6, Theorem 2]. Clearly, as both, D and $D_{i \leftarrow j}$ are consistent DAG extension of the same pattern P , $D_{i \leftarrow j}$ is Markov equivalent to D , which finishes the proof.

(b) As $G_{P,K} \neq G_{P,K \setminus \{i \rightarrow j\}}$, by Lemma 3.1 (a), there exists a consistent DAG extension of $G_{P,K}$ in which $i \rightarrow j$ is covered. From that, it immediately follows that all $k \in \text{pa}_{G_{P,K}}(i)$ are adjacent to j in $G_{P,K}$. As $G_{P,K}$ is closed under R1-R4, $k \rightarrow j$ in $G_{P,K}$ due to R2. Concludingly, $\text{pa}_{G_{P,K}}(i) \subseteq \text{pa}_{G_{P,K}}(j)$. Analogously, for $k' \in \text{pa}_{G_{P,K}}(j) \setminus \{i\}$, either $k' \rightarrow i$ or $k' - i$ in $G_{P,K}$ as $i \rightarrow j$ can be covered.

STEP 1: Orient $k' - i$ with $k' \in \text{pa}_{G_{P,K}}(j)$ into i . To be precise, define the new background knowledge $\tilde{K} := K \cup (\bigcup_{k' \in \text{pa}_{G_{P,K}}(j)} \{k' \rightarrow i\})$. As there is a consistent DAG extension D of $G_{P,K}$ in which $i \rightarrow j$ is covered, $k' \rightarrow i$ in D for all $k' \in \text{pa}_{G_{P,K}}(j) \setminus \{i\}$. Hence, by definition, \tilde{K} is consistent.

STEP 2: Close orientations under R1-R4 to obtain the maximally oriented PDAG $G_{P,\tilde{K}}$ with respect to the pattern P and background knowledge \tilde{K} [12].

Claim 1: Let (x, y, z) , $z \in \{i, j\}$ be a triple such that $x - y$ or $y - z$ in $G_{P,K}$ and $x \rightarrow y \rightarrow z$ in $G_{P,\tilde{K}}$. Then $y = i, z = j$ or $x \rightarrow y - z$ in $G_{P,K}$.

Suppose that $y \neq i$ and $x - y$ in $G_{P,K}$. Then, $x \rightarrow y$ in $G_{P,\tilde{K}}$ was oriented in STEP 2 by applying R1-R4. We will lead this to a contradiction. By Lemma A.7, y is a descendant of i in $G_{P,\tilde{K}}$. Moreover, recall that $y \rightarrow z$ in $G_{P,\tilde{K}}$. By construction, there exists a consistent DAG extension D of $G_{P,\tilde{K}}$ in which $i \rightarrow j$ is covered. As $y \neq i$ and $z \in \{i, j\}$, $y \rightarrow i$ and $y \rightarrow j$ in D . But y is a descendant of i in D , so D contains a cycle. Contradiction.

Claim 2: In STEP 2, no additional edges are oriented into i or j .

Suppose the contrary and consider the first edge that is oriented into i or j by applying one of R1-R4 in STEP 2. We will consider the rules case-by-case.

R1: Let x be the upper, y the lower left and z the right node in R1 in Figure 6. Suppose $y \rightarrow z$, $z \in \{i, j\}$ is implied by R1 in STEP 2. Thus, $x \rightarrow y \rightarrow z$ in $G_{P,\tilde{K}}$ and $y - z$ in $G_{P,K}$. As $G_{P,K}$ is closed under R1-R4, $x - y$ in $G_{P,K}$. Then, by Claim 1, $y = i$ and $z = j$. But $i \rightarrow j$ in $G_{P,K}$, contradiction.

R2: Let x be the left, y the middle and z the right node in R2 in Figure 6. Thus, $x \rightarrow y \rightarrow z$ with $x \rightarrow z$ in $G_{P,\tilde{K}}$, and $x - z$ in $G_{P,K}$.

Case 1: $y = i$. As $z \in \{i, j\}$, $z = j$. As $i \rightarrow j$ and $x - z = j$ in $G_{P,K}$ and $G_{P,K}$ is closed under R1-R4, $x - y = i$ in $G_{P,K}$. Therefore, $x \rightarrow y = i$ in $G_{P,\tilde{K}}$ was either oriented in STEP 1 or STEP 2. It was not oriented in STEP 1 as $x - z = j$ (that is, $x \notin \text{pa}_{G_{P,K}}(j)$). Also, it was not oriented in STEP 2 as by assumption, $x \rightarrow z$ is the first edge oriented into i or j in STEP 2. Contradiction.

Case 2: $y \neq i$. By Claim 1, $x \rightarrow y - z$ in $G_{P,K}$. By assumption, $x - z$ is the first edge that is oriented into $z \in \{i, j\}$ in STEP 2. Hence, $y - z$ was oriented into z in STEP 1 ($y \in \text{pa}_{G_{P,K}}(j)$) and $x - z$ not ($x \notin \text{pa}_{G_{P,K}}(j)$). As x is oriented into $z \in \{i, j\}$ in $G_{P,\tilde{K}}$ and as there is a consistent DAG extension of $G_{P,\tilde{K}}$ in which $i \rightarrow j$ is covered, $x - i$ and $x - j$ in $G_{P,K}$. Recall that $x \rightarrow y$ in $G_{P,K}$ and $y \in \text{pa}_{G_{P,K}}(j)$. As $G_{P,K}$ is closed under R1-R4, $x \rightarrow j$ in $G_{P,K}$ by R2, which

contradicts $x \notin \text{pa}_{G_{P,K}}(j)$.

R3: Does not apply. STEP 1 and STEP 2 do not create new v -structures.

R4: Let x be the upper left, y the upper right and z the lower right node in *R4* in Figure 6. We have $x \rightarrow y \rightarrow z$ in $G_{P,\tilde{K}}$ and $x - y$ or $y - z$ in $G_{P,K}$. Note that x and z are not adjacent in $G_{P,K}$ and $G_{P,\tilde{K}}$. If $y = i$, then $z = j$ and x is a parent of i but not adjacent to j in $G_{P,\tilde{K}}$. This contradicts the fact that $i \rightarrow j$ is covered in a consistent DAG extension of $G_{P,\tilde{K}}$. Hence, $y \neq i$. By *Claim 1*, $x \rightarrow y - z$ in $G_{P,K}$. As x is not adjacent to z in $G_{P,K}$, $y \rightarrow z$ in $G_{P,K}$ by *R1*, which contradicts the fact that $G_{P,K}$ is closed under *R1-R4*. This concludes the proof of *Claim 2*.

By *Claim 2*, we do not orient edges into i or j in STEP 2. Hence, by construction, $G_{P,\tilde{K}}$ satisfies $\text{pa}_{G_{P,\tilde{K}}}(i) = \text{pa}_{G_{P,\tilde{K}}}(j) \setminus \{i\} = \text{pa}_{G_{P,K}}(j) \setminus \{i\}$. By Lemma A.8, there exists a consistent DAG extension D of $G_{P,\tilde{K}}$ in which all undirected edges incident to i and j are oriented out of i and j . By construction, D is a consistent DAG extension of $G_{P,K}$. Moreover, $\text{pa}_D(i) = \text{pa}_D(j) \setminus \{i\} = \text{pa}_{G_{P,K}}(j) \setminus \{i\}$, which concludes the proof. \square

Lemma A.7. *Consider the maximally oriented PDAG $G_{P,K'}$ (with orientations closed under *R1-R4*) with respect to the pattern P and consistent background knowledge K' . Let $a_m - b$ in $G_{P,K}$ for all $1 \leq m \leq M$ and assume there exists a consistent DAG extension of $G_{P,K'}$ in which $a_m \rightarrow b$ for all $1 \leq m \leq M$. We orient $a_m \rightarrow b$ for all $m \leq M$ and close the orientations under *R1-R4*. Let us denote the edges we orient $a'_m \rightarrow b'_m$, $m = 1, 2, \dots$. Then $b'_m, m \geq 0$ are descendants of b .*

Proof. By induction. By definition, b is a descendant of b . At each step, apply one of *R1-R4* and orient $a'_m \rightarrow b'_m$. This only occurs if one of the directed edges in one of *R1-R4* is actually an edge $a_k \rightarrow b$ or $a'_k \rightarrow b'_k$ that was oriented at an earlier stage $1 \leq k \leq M$ (in the first case) or $k < m$ (in the second case). By the induction assumption, b'_k is a descendant of b for all $k < m$. By looking at Figure 6 (i.e. going through the cases *R1-R4*) we can see that in each case, b'_m is a descendant of b (in the first case) or b'_k (in the second case). Hence b'_m is a descendant of b_0 . \square

Lemma A.8. *Consider the maximally oriented PDAG $G_{P,K}$ (with orientations closed under *R1-R4*) with respect to the pattern P and consistent background knowledge K . Let $x \rightarrow y$ in $G_{P,K}$. Then, there exists a consistent DAG extension of $G_{P,K}$ in which all undirected edges incident to x and y are oriented out of x and y .*

Proof. Orient an undirected edge e incident to y out of y and close the orientations under *R1-R4*. By [12, Theorems 2 & 4] the resulting PDAG is maximally oriented with respect to the pattern P and consistent background knowledge $K \cup \{e\}$. By Lemma A.7, no edge that is oriented in that process will point into x or y . Now repeat, until there is no more undirected edge incident to y . Then, analogously orient all undirected edges incident to x out of x . \square

A.6.3. Proof of Lemma 3.2

Proof. We first prove that for $k \geq 1$, by construction, each G_{P, \mathcal{K}_k} is a consistent extension of $G_{\mathcal{D}(\mathbb{P})}$. This means that G_{P, \mathcal{K}_k} and $G_{\mathcal{D}(\mathbb{P})}$ have the same skeleton and v -structures and $i \rightarrow j$ in $G_{\mathcal{D}(\mathbb{P})} \Rightarrow i \rightarrow j$ in G_{P, \mathcal{K}_k} . Then, we show that there exists a $k_0 \leq |\mathcal{K}_1^{\text{init}}| + 1$ such that either $\mathcal{K}_{k_0}^{\text{init}} = \emptyset$ or there is no edge in $\mathcal{K}_{k_0}^{\text{init}}$ that is covered in any of the consistent DAG extensions of $G_{P, \mathcal{K}_{k_0}}$. For k_0 it holds that $G_{P, \mathcal{K}_{k_0}} = G_{\mathcal{D}(\mathbb{P})}$.

By construction, $G_{P, \mathcal{K}_1} = D^0$ is a consistent extension of $G_{\mathcal{D}(\mathbb{P})}$. By Theorem 2.2 (b), if $\mathcal{K}_1^{\text{init}} = \emptyset$ or none of the edges in $\mathcal{K}_1^{\text{init}}$ are covered in D^0 , $G_{\mathcal{D}(\mathbb{P})} = D^0 = G_{P, \mathcal{K}_1}$. For a fixed $k \geq 1$, suppose that G_{P, \mathcal{K}_k} is a consistent extension of $G_{\mathcal{D}(\mathbb{P})}$ and that there exists $\{i \rightarrow j\} \in \mathcal{K}_k^{\text{init}}$ that is covered in a consistent DAG extension of G_{P, \mathcal{K}_k} , which we denote by D . By assumption, as G_{P, \mathcal{K}_k} is a consistent extension of $G_{\mathcal{D}(\mathbb{P})}$, D is a consistent DAG extension of $G_{\mathcal{D}(\mathbb{P})}$. Hence, $D \in \mathcal{D}(\mathbb{P})$ by Theorem 2.1. Case 1: As $i \rightarrow j$ is covered and linear in $D \in \mathcal{D}(\mathbb{P})$, by Theorem 2.2 (a), there is a DAG $D' \in \mathcal{D}(\mathbb{P})$ with $i \leftarrow j$. Therefore, by Definition 2.1, $i - j$ in $G_{\mathcal{D}(\mathbb{P})}$.

By construction, $\mathcal{K}_{k+1} = \mathcal{K}_k \setminus \{i \rightarrow j\}$. Hence, by Lemma 3.1 (a), $G_{P, \mathcal{K}_{k+1}}$ equals G_{P, \mathcal{K}_k} except for an undirected edge $i - j$ (all other directed edges in G_{P, \mathcal{K}_k} are either directed in P or still contained in \mathcal{K}_{k+1} , hence they must be directed in $G_{P, \mathcal{K}_{k+1}}$). Therefore, $G_{P, \mathcal{K}_{k+1}}$ is a consistent extension of $G_{\mathcal{D}(\mathbb{P})}$.

Case 2: As $i \rightarrow j$ is covered and nonlinear in $D \in \mathcal{D}(\mathbb{P})$, by Theorem 2.2 (a), $i \rightarrow j$ in all DAGs in $\mathcal{D}(\mathbb{P})$. Hence, $i \rightarrow j$ in $G_{\mathcal{D}(\mathbb{P})}$ by Definition 2.1.

By construction, $\mathcal{K}_{k+1} = \mathcal{K}_k$ and $G_{P, \mathcal{K}_{k+1}} = G_{P, \mathcal{K}_k}$ is a consistent extension of $G_{\mathcal{D}(\mathbb{P})}$. Moreover, as $\{i \rightarrow j\} \notin \mathcal{K}_{k+1}^{\text{init}}$ and $\{i \rightarrow j\} \in \mathcal{K}_{k+1}^{\text{nonl}}$, $i \rightarrow j$ is fixed in all G_{P, \mathcal{K}_l} for $l > k$.

In both cases, $|\mathcal{K}_{k+1}^{\text{init}}| = |\mathcal{K}_k^{\text{init}}| - 1$. Hence, there exists a $k_0 \leq |\mathcal{K}_1^{\text{init}}| + 1$ such that either $\mathcal{K}_{k_0}^{\text{init}} = \emptyset$ or no edge in $\mathcal{K}_{k_0}^{\text{init}}$ is covered in any of the consistent DAG extensions of $G_{P, \mathcal{K}_{k_0}}$. We will now prove that $G_{P, \mathcal{K}_{k_0}} = G_{\mathcal{D}(\mathbb{P})}$. If $\mathcal{K}_{k_0}^{\text{init}} = \emptyset$, this immediately follows from Case 1 and Case 2. For $\mathcal{K}_{k_0}^{\text{init}} \neq \emptyset$, suppose $G_{P, \mathcal{K}_{k_0}} \neq G_{\mathcal{D}(\mathbb{P})}$. Then, there are $M \geq 1$ edges $i_m \rightarrow j_m, m = 1, \dots, M$ in $G_{\mathcal{D}(\mathbb{P})}$ with $i_m \rightarrow j_m$ in $G_{P, \mathcal{K}_{k_0}}$. By construction, $\{i_m \rightarrow j_m\}_{m=1, \dots, M} \subseteq \mathcal{K}_{k_0}$. From Case 2 it must hold that $\{i_m \rightarrow j_m\}_{m=1, \dots, M} \subseteq \mathcal{K}_{k_0}^{\text{init}}$. By Theorem 2.2 (b), $\mathcal{D}(\mathbb{P})$ is connected with respect to covered linear edge reversals. Hence, there exists an $1 \leq m_0 \leq M$ for which $i_{m_0} \rightarrow j_{m_0}$ is covered in a consistent DAG extension of $G_{P, \mathcal{K}_{k_0}}$. But $\{i_{m_0} \rightarrow j_{m_0}\} \in \mathcal{K}_{k_0}^{\text{init}}$, contradiction. We just showed that $G_{\mathcal{D}(\mathbb{P})}$ is a consistent extension of $G_{P, \mathcal{K}_{k_0}}$. As by construction, $G_{P, \mathcal{K}_{k_0}}$ is a consistent extension of $G_{\mathcal{D}(\mathbb{P})}$, we conclude that $G_{P, \mathcal{K}_{k_0}} = G_{\mathcal{D}(\mathbb{P})}$, which finishes the proof. \square

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